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# **Unified Very Low Stratus Cloud/Subcloud Microphysics Model: User's Guide**

by **Neal H. Kilmer**  
**Physical Science Laboratory**

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13. ABSTRACT (Maximum 200 words) Use of computer program MACACASM is described. MACACASM is based on the Raabe-Kilmer microphysics model for simulating very low stratus clouds and their associated subcloud regions. This model uses the assumption that the atmosphere contains particles that grow in the presence of moisture as a function of relative humidity, temperature, and the size and chemistry of the particles. Components of this model include droplet growth and evaporation, phase change and mass balance of total water, thermodynamics, and ascent of a cluster of drops enclosed in moist air. User input includes some conventional meteorological values at a reference height near ground level and some parameter values and other specifications. Vertical profiles of drop size distributions can be simulated and used for further analysis. Examples of further use of drop size distribution profiles include simulation of profiles of extinction, backscatter, absorption, and scattering coefficients. The first part of this guide is intended for the scientist-user. The second part has been prepared for the computer programmer who may be developing other programs related to this model.					
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# 1. Introduction

The Rachele-Kilmer microphysics model for very low stratus clouds and subcloud regions is a largely theoretically based model, in contrast to current empirically based models. The Rachele-Kilmer model is described in a detailed technical report, [1] which may be consulted for assumptions that compose the model and for mathematical details. Some profiles simulated for very low stratus clouds using this model were compared with profiles calculated using actual field data. [1]

Use of the Rachele-Kilmer microphysics model for very low stratus clouds and subcloud regions is enabled by computer program MACACASM, the source code for which has been stored in file ~nkilmer/sources/hp\_macacasm.f for use with Hewlett-Packard 9000 computers at U.S. Army Research Laboratory (ARL) West. MACACASM is an acronym for Microphysics and Cluster Ascent Cloud and Subcloud Model. This program and the other programs described in this guide are written in Fortran 77.

Certain output files may be used with Mie calculations or stored Mie efficiency factors to simulate vertical profiles of extinction, backscatter, scattering, and absorption coefficients. This capability requires use of one or two other programs also. Details are given in sections 5.0, 5.1, and 5.2.

This guide for using the computerized model is in two parts to separate the material required by two different types of users. The first part (sections 2 through 6) is intended for the scientist-user. It assumes an understanding of meteorological theory and experience with analysis and modeling of meteorological data, but no programming skills beyond basic computer literacy. The second part (section 7) has been prepared for the computer programmer who may be developing other programs related to this model.

NOTE: MACACASM is a research mode program. It is possible for the user to supply sets of input values that are not self-consistent. It is up to the user to provide logically consistent input.

## 2. Input Required to Define Model

MACACASM is designed for interactive use and prompts the user for required input. The program can be run in batch mode using a redirected input file to replace interactive input. (See 2.1.4 for an example of such a file.)

When using MACACASM in interactive mode, the user must indicate choices when prompted. The user may specify additional input (without being prompted) by supplying it in input files `.haze.defaults` and `zbase_b_c.in`. If these files and the information expected to be in them are not found, default values will be used.

User input, required to execute the current models, includes the following:

- a method of specifying concentrations of all sizes of droplets at the reference height and the radii of the corresponding dry nuclei (see below)
- specification of how the droplet number concentration varies with height (inversely proportional to the volume of the cluster sphere in the most common usage)
- reference height
- relative humidity, pressure, and temperature in the cluster sphere, and temperature in the ambient environment at the reference height
- type of nucleus (preferably one of the ten reported by Hänel and Lehmann [2])
- ascent rate and radius of the cluster sphere at the reference height
- an entrainment parameter
- the height of the top of the cloud.

In addition, the user specifies a value that affects precision of calculations: the height step used in numerical integration.

Optional input includes some constants in the temperature lapse rate equation for modifying modeled behavior near the base of an inversion, which is typically modeled as occurring at the same height as the top of the cloud. If the user does not provide values for those constants, default values are used.

Also optional is the inclusion of a term that is linear with height above the reference height in the temperature lapse rate equation for the ascending cluster sphere. The term may be used to model effects not otherwise modeled, including radiation effects. Positive values of the constant coefficient (alapslin) in the term tend to decrease values for liquid water content compared with what they would be at the same height when the term is not present (or when its constant coefficient is zero). The latter-mentioned case has been called quasi-adiabatic. Negative values of the constant coefficient tend to increase corresponding values for liquid water content. If the constant coefficient is not provided, it is considered to be zero. Use of the constant coefficient is discussed in a later paragraph.

The entrainment parameter is used in modeling horizontal entrainment from the ambient environment at the same height as the cluster sphere. If a value of zero is specified, there is an option for providing values of constants to be used in modeling turbulent transfer of heat, momentum, and water vapor. If the latter constants are not provided, they are considered to be zero.

The usual method for specifying concentrations of droplets at the reference height and the radii of the corresponding dry nuclei is as follows:

- User input values for the visibility (meteorological range) at the reference height and the number of droplet size classes are required in addition to the input specified above.
- The visibility and relative humidity are used to define the parameters of a Shettle-Fenn [3] bimodal lognormal distribution at the reference height.

- A lower dry particle (condensation nucleus) size limit is set. The value is used to calculate the lower limit for droplet size at the reference height.
- Because some of the Shettle-Fenn distribution is not used, the input value of the visibility is expected to be smaller than the observed (or desired) meteorological range (visibility) at the reference height. To maintain self-consistency, the user is given the option of dividing each of the N1 and N2 parameters of the original Shettle-Fenn distribution by a constant. The same constant is typically chosen for use with N2 as with N1, and the value selected is such that the calculated visibility (meteorological range) at the reference height equals the input value (to within a small roundoff error).
- For each size class, the droplet concentration and representative droplet radius are calculated by integrating an appropriate range of the distribution function and calculating the mean volume droplet radius for that range, respectively. Radii of the dry nuclei are calculated by assuming that all of the droplets at the reference height are in equilibrium with water vapor in air in the cluster sphere and using an equilibrium droplet radius equation based on Hänel and Lehmann's work [2] for the type of nucleus selected.

Sometimes it is desired to specify the value for the maximum liquid water content in terms of a percent of the quasi-adiabatic (100 percent) value that is obtained if all of the other input parameters are the same. This percent cannot be specified directly as an input value. However, the maximum liquid water content depends strongly on the value of the parameter `alapslin`, which is the coefficient of the difference  $z - z_{low}$  (that is, height minus reference height, both expressed in units of cm) in the cluster sphere lapse rate equation. This parameter is not requested interactively; rather, it is expected to be in input file `zbase_b_c.in`. The quasi-adiabatic results can be simulated by using a value of zero for the `alapslin` parameter. Then nonzero values may be used for the `alapslin` parameter in subsequent simulations. That parameter can be refined iteratively until the maximum liquid water content is sufficiently close to the desired percent of the corresponding quasi-adiabatic value.

## 2.1 Examples of Input Files

In lines containing arrows in the examples, only the input to the left of the arrows is read by the program. The arrows and the text to the right of the arrows are included for understanding but are ignored by the program. Some of this text refers to the variables  $z$  the height (cm) above ground level,  $z_{low}$  the reference height (cm) above ground level, and  $T$  the temperature (K) inside the cluster sphere.

NOTE: If standard input is to be written into a file for use as redirected input, it should be noted that the exact form of this file depends on the options selected. For example, if a Shettle-Fenn distribution is chosen to define the drop size distribution at the initial (reference) height, more lines of input are required to provide the information needed to evaluate the distribution parameters than if a Duncan-Low distribution were chosen. Also, if a suggested value is declined, an extra line is required to provide the desired input value.

The example of standard input (collected into a file for use as redirected input) includes two instances (pressure at reference height and initial effective vertical velocity) in which the default values are declined and the entered values are identical to the defaults. This practice provides an explicit record of the input values used and makes it easier for the user to modify copies of the standard input file for cases in which the default values are not the desired ones.

### 2.1.1 *Input File Named `zbase_b_c.in` for Typical Usage*

5.00E+02	← $z_{base}$ , base of INVERSION in sphere lapse rate equation in meters
1.0E+04	← $b_{hbeqn}$ , $b$ in extra term in sphere lapse rate equation
2.0E-07	← $c_{hbeqn}$ , $c$ in extra term in sphere lapse rate equation
6.5843E-10	← $a_{lapslin}$ , coeff of $(z - z_{low})$ in sphere lapse rate equation
0.0	← $c_{lturb}$ , a form factor to multiply $KK1_{turb}$
0.0	← $c_{2turb}$ , a form factor to multiply $KK2_{turb}$
0.0	← $c_{3turb}$ , a form factor to multiply $KK3_{turb}$
0.0	← $KK1_{turb}$ , the turbulent transfer coefficient for momentum

0.0            ← KK2tur, the turbulent transfer coefficient for heat  
 0.0            ← KK3tur, the turbulent transfer coefficient for water vapor  
                  mixing ratio

### 2.1.2 *Input File Named zbase\_b\_c,in with Priestley-Type Constants*

5.00E+02      ← zbase, base of INVERSION in sphere lapse rate equation in  
                  meters  
 1.0E+04      ← bhbeqn, b in extra term in sphere lapse rate equation  
 2.0E-07      ← chbeqn, c in extra term in sphere lapse rate equation  
 6.5843E-10   ← alapslin, coeff of (z-zlow) in sphere lapse rate equation  
 8             ← c1tur, a form factor to multiply KK1tur  
 8             ← c2tur, a form factor to multiply KK2tur  
 8             ← c3tur, a form factor to multiply KK3tur  
 30            ← KK1tur, the turbulent transfer coefficient for momentum  
 18            ← KK2tur, the turbulent transfer coefficient for heat  
 30            ← KK3tur, the turbulent transfer coefficient for water vapor  
                  mixing ratio

### 2.1.3 *Input File Named .haze.defaults*

10000        ⇐ plot\_interval in units of 0.1 mm  
 100000      ⇐ writ\_interval in units of 0.1 mm

### 2.1.4 *Standard Input Collected Into a File for Use as Redirected Input*

2             ← moderate amount of output  
 5             ← Shettle-Fenn distribution for droplets at reference height  
 2             ← maritime air mass  
                  ← Blank line is interpreted as "yes": Use divisors of N1  
                  and N2.  
 0.953773     ← divisor of original Shettle-Fenn parameter N1  
 0.953773     ← divisor of original Shettle-Fenn parameter N2  
 4.0E-03      ← lower cutoff ( $\mu\text{m}$ ) for dry radii

4	← drop concentration is inversely proportional to sphere volume.
n	← no drop fallout
0.01	← entrainment parameter
2	← reference (initial) height (m)
5.0	← visibility (km) at reference height
550	← maximum height (m) for simulation
n	← This is not top of cloud.
500	← height (m) of top of cloud
0.1	← height increment (m)
n	← Do not automatically accept default nucleus type.
20	← nucleus type
n	← Decline default relative humidity at reference height.
0.95	← relative humidity at reference height
n	← Decline default pressure at reference height.
1000	← pressure (mbar) at reference height
n	← Decline default reference height temperature in cluster sphere.
288.6827	← reference height temperature in cluster sphere
n	← Decline default reference height temperature of ambient environment.
288.15	← reference height temperature of ambient environment
	← Blank line is interpreted as "yes": Keep number of drop sizes.
3	← method for determining effective vertical velocity of sphere
n	← Decline default initial effective vertical velocity of sphere.
3	← initial value (cm/s) for effective vertical velocity of sphere
200	← sphere radius (cm) at reference height
n	← dT/dz in cluster sphere is not to be treated as known.
-1	← Use default droplet radii to define size class boundaries.

← Blank line: Yes, accept initial volume of condensed matter.

## **2.2 Questions That Can Be Answered Yes or No**

Answer questions that can be answered yes or no by entering the first letter (y or n) of the desired response.

NOTE: Avoid entering anything, including a blank, before the desired y or n. The first character entered, including a blank, enter, or return, is considered a yes answer unless the character is n or N.

## **2.3 In Case of an Unacceptable Entry in Standard Input**

A common response to an unacceptable entry in standard input is

Unrecognized option. Please try again.

If running the program interactively, enter revised input appropriate for the last prompt that required input and continue as prompted. However, if standard input is being supplied by a redirected input file, the program is not expected to run properly after the message is encountered. In the latter case, output files resulting from the run in which the error message was generated should be deleted, and the file being used as standard input should be edited to change the unacceptable input to acceptable input. The program should be executed again from the beginning.



### 3. Example Dialogue Between MACACASM and a User

This section contains examples of interactive dialogue between MACACASM and a user. In general, the examples are chronologically arranged as they occur during an execution of the program. As indicated in this report, the presence or absence of some dialogue depends on one or more choices made by the user.

Between the end of this paragraph and the end of 3.29, text printed in this font represents text written to standard output during execution of MACACASM. Unless standard output is redirected, the text is expected to appear on the terminal screen. When user choices result in such text being skipped, as indicated by "Skip to ..." or similar wording, the text does not appear on the terminal screen.

Text printed in this font is for explanation, clarification, etc., and does not appear on the terminal screen during execution of the program.

#### 3.1 Level of Output Desired

Indicate level of output desired:

- (1) data files only,
  - (2) data files plus some text (not much for each drop size class), or
  - (3) data files plus much text, including values for each size class.
- Enter 1, 2, or 3 →

The user's choice greatly affects the amount of text to be written into output file haze.out, which is an output text file suitable for printing in a 132-column format. This choice does not affect the existing content of data files suitable for use with plot software.

Text will be written into output file "haze.out".

#### 3.2 Method of Specifying Dry Radii

Indicate method of specifying dry radii:

- (1) User specifies each dry radius and each number of droplets;
- (2) User specifies each droplet radius at reference height and each number of droplets;

(4) Duncan-Low distribution is used for droplet radii at reference height, and boundaries of droplet size intervals are set by user or calculated; or

(5) Shettle-Fenn distribution is used for droplet radii at reference height, and boundaries of droplet size intervals are set by user or calculated.

The relative humidity at reference height is used in calculating dry radii in methods 2, 4, and 5.

Enter the desired method (1, 2, 4, or 5) →

(Method 3 has been eliminated.)

Dry radii (equivalent sphere radii of dry condensation nuclei) are calculated or specified at the initial (reference) height. The dry radii are used during the simulation, except when the associated droplets are removed by gravitational settling. If method 1 is selected, the dry radii can be specified directly (default values also available). If another method is selected, a set of droplet (wet) radii is calculated or specified at the initial height and used with the relative humidity to determine the set of dry radii by assuming that the droplets are perfect spheres at their equilibrium sizes. If method 2 is selected, the initial droplet radii and concentrations can be specified directly (default values also available).

Methods 4 and 5 define a continuous drop size distribution at the initial (reference) height and represent this distribution by a discrete drop size distribution at that height. To define the discrete distribution, the radius ranges of a number of bins (intervals) equal to the desired number of size classes are specified. It is convenient to define one lower cutoff value and let the program calculate the remaining ranges. A representative radius is calculated for each bin (range or interval). Because of the importance of volume in calculating liquid water content, the mean volume drop radius in a given interval is used as the representative radius for that interval. For each size class, the initial drop concentration and the representative drop radius are determined by integration, with respect to drop radius, using the drop size distribution expressed as a function of drop radius.

The continuous drop size distribution type used at the initial (reference) height may be different depending on the method. If method 4 is selected, a

Duncan-Low distribution is used for droplet radii at the initial height. The distribution is a bimodal gamma distribution, parameters of which are functions of visibility. If method 5 is selected, a Shettle-Fenn distribution is used for droplet radii at the initial height. A Shettle-Fenn distribution is a bimodal lognormal distribution, of which parameters are functions of visibility and relative humidity.

If method 1 or 2 is selected, skip to 3.5.

If method 4 is selected, skip to 3.4.

### 3.3 If Method 5 is Selected

If method 5 is selected, the following prompts appear in standard output (on terminal screen if program is being run interactively):

```
Specify which Shettle-Fenn model is to be used,  
(1) rural,  
(2) maritime, or  
(3) urban.  
Enter number of desired model (1, 2, or 3) →
```

The user is presented with a choice of three air mass types (maritime, rural, and urban) and is asked to select one. Near a coastline with wind blowing in from the ocean, a maritime air mass is the appropriate selection. In a city, an urban air mass is appropriate. Inland and not near a city, a rural air mass is appropriate.

```
Do you want to divide at least one of the Shettle-Fenn  
parameters N1 and N2 by a constant (yes or no)?
```

Answer y or n.

Sometimes the visibility, calculated as  $(LN\ 50)/(\text{extinction coefficient, km}^{-1}, \text{ for } 550\text{ nm wavelength})$ , does not agree exactly with the input value at the initial (reference) height. Agreement can be forced by adjusting the original Shettle-Fenn parameters N1 and N2, which are used to specify the concentrations of droplets associated with the respective modes. If such

adjustment is necessary, N1 and N2 should be divided by the same constant. Although the capability exists for entering different values for the two divisors, unequal values do not preserve the shape of the unaltered Shettle-Fenn drop size distribution. If the preceding question was answered yes, the user is prompted for values of constants as follows:

Enter positive constant used to divide N1 →  
Enter positive constant used to divide N2 →

### **3.4 Lower Cutoff for Dry Particle Radius**

Please define lower cutoff: Enter smallest dry particle radius (in micrometers) to be allowed (or 0 for no cutoff) →

Because of the kelvin cutoff, extremely small droplets are not expected to become activated in typical cloud and subcloud conditions. The impact of such small droplets on usual quantities of interest, such as total liquid water content and extinction, is expected to be minuscule. Also, numerical difficulties may be encountered when attempting to determine an equilibrium radius (droplet radius when the dry radius is known or vice versa) at a given relative humidity. Other factors being equal, the ratio of wet radius to dry radius at the point of critical supersaturation tends to be smaller for smaller condensation nuclei. For extremely small nuclei, the ratio could be smaller than the ratio used in this software to define an initial guess for the equilibrium (droplet or dry) radius. With the initial guess being on the wrong side of the maximum of the Kohler curve, the solution algorithm might continue to change trial radius values in the wrong direction until a trial radius value is so huge or tiny that the program aborts. Therefore, a lower cutoff is used for the dry particle radius. A typical value used for this cutoff is 0.004  $\mu\text{m}$ .

### 3.5 Number of Droplets Definition Option

Do you want the number of droplets per cubic centimeter (except as modified by droplets falling out) to be

- (1) constant,
- (2) proportional to the density of dry air,
- (3) read from binary data file "drop.conc.in", or
- (4) inversely proportional to cluster sphere volume, which depends on density in cluster sphere

(Enter 1, 2, 3, or 4)?

The user's choice here is called the "Number of Droplets Definition Option" later in this documentation.

Option 1 is a simple approximation. It is not strictly consistent with a fixed number of droplets in an expanding sphere.

Option 2 is a reasonable approximation of the effect of expansion on the droplet concentration.

Option 3 gives the user increased flexibility. However, care should be taken to avoid internal inconsistencies when modeling with this option.

Option 4 is appropriate if the droplet concentration is modeled as though the droplets were evenly distributed throughout the sphere but do not pass through the surface of the sphere. This is the option typically used. It is also the only option (of these four) with which the user also is allowed to set the value of an entrainment parameter.

Because the radius of the cluster sphere is modeled as being inversely proportional to the cube root of the partial density of dry air in the cluster sphere, options 2 and 4 seem to represent very similar effects on the number of droplets per cubic centimeter. Again, note that Option 4 is also the only option (of these four) with which the user also is allowed to set the value of an entrainment parameter.

Unless option 3 is selected, skip to 3.7.

### 3.6 Option 3 Only

If the user chooses Number of Droplets Definition Option 3, the file drop.conc.in must be available as an input file in the connected directory. The file must be unformatted (binary) and sequential, and it must contain one record for every height level used in numerical integration. (The first record is for the initial height, the second record is for the initial height plus the height increment entered by the user, and so forth.) Each record must contain the height (cm) above ground level followed by the concentrations (droplets/cm<sup>3</sup>) of droplets in all of the individual size classes in order (starting with size class 1, followed by size class 2, and so on). Each height read from this file is compared with the current height being used in model execution. If there is disagreement (allowing for reasonable tolerance), execution of the model program aborts.

### 3.7 Drop Sedimentation

Do drops fall out of cluster sphere when their settling velocities exceed the ascent velocity of this sphere?

Answer y or n.

Inclusion of this option was a first-order attempt to model effects of sedimentation, or gravitational settling, of drops. If the user answers yes, all drops in a size class are modeled as falling out of the cluster sphere when the sedimentation velocity exceeds the ascent velocity of the sphere. The drops are modeled as disappearing. There is no provision for modeling incoming drops that have fallen out of preceding spheres. This question typically is answered no.

Unless the Number of Droplets Definition Option 4 was selected, skip to 3.9.

### 3.8 Entrainment

The entrainment parameter  $\alpha$  can be nonzero only if the Number of Droplets Definition Option 4 has been selected.

**ENTRAINMENT:**

- If the entrainment parameter ALPHA is positive, it will be used, and the Priestley parameters will be set to zero.
- If ALPHA is zero, the Priestley parameters will be used if present in file "zbase\_b\_c.in".
- Negative values are not allowed for ALPHA.

Enter entrainment parameter ALPHA. →

Turbulence effects, including both entrainment and shedding, can be represented by expressions like (and one analogous to) those given by Priestley. [4] Priestley-type expressions or traditional entrainment expressions involving the entrainment parameter  $\alpha$  may be used, but do not use both. (The entrainment parameter  $\alpha$  is represented as  $\alpha_e$  in a detailed technical report [1] describing this model.)

One or neither of the two options presented may be chosen; however, the two options represent such similar, or related, effects that they must not be used simultaneously. A small entrainment effect typically is chosen by giving  $\alpha$  a small positive value (such as 0.01). Including a significant entrainment effect affects some of the model output and causes it to be different from what is expected for a well-mixed system containing only one regime throughout. For example, the simulated temperature lapse rate may be superadiabatic.

If a positive value is entered for  $\alpha$ , this message appears:

Priestley parameters are set to zero.

If zero is entered for  $\alpha$ , values of turbulent transfer coefficients and form factors for momentum and heat according to Priestley [4] and analogous parameters for water vapor mixing ratio can be used if they have already been read from file zbase\_b\_c.in. Early in the execution of the program, there is an attempt to read from the file. Existence of the file is optional; however, the default value of zero is used for each of the turbulent transfer coefficients and form factors if the file does not exist. An example of a file containing nonzero values for Priestley-type turbulent transfer coefficients is given in section 2.1.2.

### **3.9 Initial Height**

What is the initial height in meters above ground level?

The user response defines the height of the center of the cluster sphere at the beginning of the simulation. Typically, 2 m is used.

### **3.10 Initial Visibility**

What is the visibility in kilometers at the initial height?

If the initial drop size distribution is defined by a Duncan-Low or Shettle-Fenn distribution, the user-specified visibility is used in defining parameters of that distribution.

### **3.11 Height Limit and Height of Top of Cloud**

What is the final height in meters above ground level?

It is recommended to use a value a little higher than the desired top of the cloud.

Does the top of the cloud occur at this height?

Answer y or n — n if previous recommendation is followed. If the answer is n, the following prompt appears.

Enter height of top of cloud in meters above ground level →

Enter the height.

### **3.12 Height Increment**

What is the height increment in meters?

This is the height step size to be used in model calculations. Using smaller step sizes requires more computation time and leads to more accurate results. The height step size should be such that the intervals for writing output into



text file haze.out (default interval = 10 m) and plot data into various files (default interval = 0.2 m) are each an exact multiple of the height step size (the height step size multiplied by some positive integer, which could be 1). The default values for the intervals are overridden if file .haze.defaults exists and contains two integers; one integer in each of two lines. The first integer is the interval (in units of 0.1 mm) for writing plot data into various files, and the second integer is the interval (in units of 0.1 mm) for writing output into text file haze.out. Considering the units used, it is appropriate to divide both of the integers by 10,000 to compare with the value entered via standard input for the height increment in meters. In high-accuracy research mode, step sizes of 0.1 m are often used if the top of the cloud is set at 500 m or lower, and step sizes of 0.2 and 0.25 m are often used if the top of the cloud is set at 1000 m.

### 3.13 Type of Nucleus

Keep type of nucleus (14)?

Answer y or n. If the answer is y, the default nucleus indicated by the number in parentheses is used. If the answer is n, the user is presented with the following list of available choices.

Enter type:

- 1-5) not used
- 6) Hanel: NaCl
- 7) Hanel: (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>
- 8) Hanel Model 1: rural, summer 1966, Mainz
- 9) Hanel: urban, Jan 1970, Mainz
- 10) Hanel Model 6: rural
- 11) Mizpeh Ramon, Israel; desert, normal conditions
- 12) Mizpeh Ramon, Israel; desert, sand storm
- 13) Mainz, Germany; industrial
- 14) West Coast of Ireland; maritime
- 15-20) Deuselbach, Germany; background, combined with particles from surrounding industrial zones and local sources

→

Enter the integer corresponding to the desired nucleus type. The nucleus type chosen affects values of parameters used in modeling microphysics of droplet growth and evaporation. For nucleus types 11 through 20, subtract 10 to obtain the corresponding sample number reported by Hänel and Lehmann. [2]

It is suggested that the nucleus type selected be consistent with the air mass type selected. Combinations of air mass type and nucleus type that have been used include: rural air mass with nucleus type 17, maritime air mass with nucleus type 14 or 20, and urban air mass with nucleus type 13.

### 3.14 Some Initial (Reference) Height Values

Relative humidity, total pressure, and temperatures of cluster sphere and ambient environment at reference height:

Keep relative humidity ( .98000 )?

Answer y or n. If the answer is y, the number in parentheses is used. If the answer is n, the user is prompted to enter the desired relative humidity:

Enter relative humidity →

Enter the desired relative humidity (using a scale on which saturation is exactly 1) at the initial (reference) height.

Keep total pressure ( 1000.0 millibars)?

Answer y or n. If the answer is y, the number in parentheses is used. If the answer is n, the user is prompted to enter the desired total pressure at the initial (reference) height:

Enter total pressure in millibars (hectopascals) →

Enter the desired value for this pressure.

Keep cluster temperature ( 273.16 K )?

Answer y or n. If the answer is y, the number in parentheses is used. If the answer is n, the user is prompted to enter the desired cluster temperature at the initial (reference) height:

Enter cluster temperature in degrees kelvin →

Enter the desired value for the temperature.

Keep temperature of ambient environment ( 273.16 K )?

Answer y or n. If the answer is y, the number in parentheses is used. If the answer is n, the user is prompted to enter the desired temperature of the ambient environment immediately outside of the cluster sphere at the initial (reference) height by:

Enter temperature of ambient environment  
in degrees kelvin →

Enter the desired value for the temperature.

### 3.15 Number of Droplet Sizes

Keep number of droplet sizes ( 80 )?

Answer y or n. If the answer is y, the number in parentheses is used. If the answer is n, the user is prompted to enter the desired number of droplet sizes:

Enter new number →

Enter the desired number of droplet sizes. If the input number is too large for the allotted array sizes, it will be changed to the maximum allowed value, and a message will be written. An example of such a message generated when the maximum allowed value is 80 follows:

```
*** Owing to limit on number of partitions,  
    this quantity has been reset to 80.
```

### 3.16 Effective Vertical Velocity of Cluster Sphere

Choose method for determining effective vertical velocity of cluster:

Effective vertical velocity of cluster is to be

- (1) constant (value entered by user),
- (2) read from file eff\_vert\_v.in,
- (3) calculated using cluster sphere buoyancy, or
- (4) calculated as a linear function of height.

Enter 1, 2, 3, or 4 →

Method 3 typically is used.

Unless method 2 is chosen, skip to 3.18.

### 3.17 If Vertical Velocity is to be Read from a File

If the effective vertical velocity is to be read from file `eff_vert_v.in` (method 2), the file must be available in the connected directory. The file is expected to be an ASCII file with each line containing three floating-point numbers. The exact format used to express each number is not critical as long as the numbers are in the expected sequence and can be read properly using a free-format read statement. The sequence for each line is expected to be: height (cm) above ground level, total elapsed time (s), and effective vertical velocity of cluster sphere (cm/s) at the listed height. The second number is read and ignored; however, the first and third values are used, so the numbers must be in the proper sequence. The height values must be identical (within reasonable tolerance) to the heights of the levels used in model calculations within the program. If there is a disagreement in the height value, the program aborts with the following message:

```
STOP Unexpected height encountered in file eff_vert_v.in
```

To ensure that the heights of file `eff_vert_v.in` correspond with the numerical integration height levels, the initial height given in the file must correspond with the value entered interactively (or in a redirected standard input file) for the initial height in meters above ground level (notice the units) when running the Rachele-Kilmer microphysics model program (for example, 200 cm and 2 m, respectively). Also, the height interval (difference in height values in consecutive lines) in file `eff_vert_v.in` must correspond with the value entered interactively (or in a redirected standard input file) for the height increment in meters (for example, 10 cm and 0.1 m, respectively).

Note that the structure expected for file `eff_vert_v.in` is exactly the same as that used for the output file `eff_vert_v.out`. This relationship could help a researcher study the effect of varying only one variable. This researcher might initially choose method 3 for determining the effective vertical velocity, while making sure that the first number in file `.haze.defaults` is exactly 10,000 times the value that is to be entered interactively (or in a redirected standard input file) for the height increment in meters (for example, 1000 and 0.1, respectively) in subsequent runs. (The height interval of output in file

eff\_vert\_v.out and a number of other output data files is determined by the first number in file .haze.defaults if that file exists. However, the height increment for numerical integration is determined by the user response when prompted for the height increment in meters. The two intervals are not automatically equal.) The researcher could copy the output file eff\_vert\_v.out to file eff\_vert\_v.in in the appropriate directory and use this copy with subsequent runs.

Skip to 3.19.

### **3.18 Initial or Constant Value for Effective Vertical Velocity**

Keep effective vertical velocity ( 3.0000000 cm/sec )?

Answer y or n. If the answer is y, the value in parentheses is used for the initial effective vertical velocity of the cluster sphere. If the answer is n, the user is prompted to enter the desired value:

Enter initial value (in cm/sec) for effective  
vertical velocity of cluster →

for method 3 or 4 for determining effective vertical velocity, or

Enter constant value (in cm/sec) for effective  
vertical velocity of cluster →

for method 1.

Enter the requested value for the initial (or constant) effective vertical velocity of the cluster sphere.

### **3.19 Initial Value for Radius of Cluster Sphere**

Enter radius (in cm) of cluster sphere at reference height →

This radius typically is set equal to the initial (reference) height above ground level. Note that the units of the input values are different for these two entries (meters for initial height and centimeters for the initial radius of cluster

sphere). Typical values are 2 m for the initial height and 200 cm for the radius.

### 3.20 Vertical Gradient of Temperature in Cluster Sphere

Is  $dT/dz$  in cluster sphere to be treated as known?

Answer y or n. N typically is entered, in which case the following message is written:

Both  $dT/dz$  and mass loading initially are unknown in cluster sphere. An equation from thermodynamics and the ideal gas law is added in order to determine both  $dT/dz$  and  $d(\text{water vapor mixing ratio})/dz$  as unknowns in this sphere.

If n is entered, skip to 3.22.

### 3.21 If User Elects to Specify $dT/dz$ Profile

What method is to be used to determine  $dT/dz$  in cluster sphere,  
(1) moist adiabatic approximation,  
(2)  $dT/dz$  = constant defined by user, or  
(3) calculation from function  $dtdzfn$ ?  
Enter 1, 2, or 3 →

#### 3.21.1 *If Method 1 (Moist Adiabatic Approximation) Is Selected*

Moist adiabatic approximation will be used.

This message confirms the selection. The value of the vertical gradient of temperature in the cluster sphere is calculated automatically at each height using the moist adiabatic approximation.

This option seems applicable within a cloud or layer of fog; however, it is not recommended for modeling the subcloud region.

Skip to 3.22.

### **3.21.2 *If Method 2 ( $dT/dz = \text{Constant Defined by User}$ ) Is Selected***

Enter value for  $dT/dz$  in cluster sphere:

Enter a floating-point number for the constant value of the vertical gradient of temperature in the cluster sphere (in units of kelvin per cm). A negative number is used to model the usual situation of temperature decreasing with height.

The option (constant  $dT/dz$  throughout entire height range) is not recommended if both subcloud and in-cloud regions are to be modeled, as the temperature lapse rate within the cloud is expected to be different from that beneath the cloud.

Skip to 3.22.

### **3.21.3 *If Method 3 (Calculation from Function $dtdzfn$ ) Is Selected***

This option allows the advanced user to supply a customized subprogram defining the behavior of  $dT/dz$  in the cluster sphere as a function of height. This may be done by replacing the Rachele-Kilmer microphysics model program's  $dtdzfn$  function subprogram and recompiling (with a Fortran 77 compiler) and loading the entire program. The  $dtdzfn$  function subprogram must have the same name, define a real\*8 function in Fortran 77, and have exactly one formal parameter that is a real\*8 variable to represent height (cm) above ground level. The values of the formal parameter and the variables in common must not be changed in the function subprogram. An example of such a function subprogram is given:

```
real*8 function dtdzfn (zcm)
```

```
* Function to calculate  $dT/dz$  (in units of degrees kelvin per cm)
* given z (height above ground in cm)
* This could be replaced by a user-defined function by replacing
* this function subprogram with an "include" statement used to
* insert a file containing a user-defined function having the same
* name, type, and formal parameter.
```

```

implicit none

* ... /params/ common block:

real*8 ahanel, bhanel, denH2O, dryvol, dtdz,
& eta, etazero, fsave, fzero, kay, lzero, msoverm0, rdry,
& rhozero, Rvapor, sigma, sigmaw, spvolH2O, theta, tzero

integer nuctype

common /params/ ahanel, bhanel, denH2O, dryvol, dtdz,
& eta, etazero, fsave, fzero, kay, lzero, msoverm0, rdry,
& rhozero, Rvapor, sigma, sigmaw, spvolH2O, theta, tzero,
& nuctype

* ... /param2/ common block:

integer dtdzmeth, nodmode

real*8 Cp, CpliqH2O, Cpvapor, dlnfdz, dqdz,
& eff_vert_v, epsilon, grvcgs, klwater, latenthv, mixrat,
& mwH2O, pdry, pdynes, pi, pwater, rdcgs, rhoacgs, spechum,
& thetam, zlow

common /param2/ Cp, CpliqH2O, Cpvapor, dlnfdz, dqdz,
& eff_vert_v, epsilon, grvcgs, klwater, latenthv, mixrat,
& mwH2O, pdry, pdynes, pi, pwater, rdcgs, rhoacgs, spechum,
& thetam, zlow, dtdzmeth, nodmode

real*8 zcm

if (zcm .le. 1600.01d+00) then
  dtdzfn = -0.1082d+00 / zcm
else
  dtdzfn = -0.2485d+00 / zcm
end if

return
end

```

In this example, none of the variables available through labeled common are used in calculating the value of dtdzfn. However, the values are being made available in case the user wants to use them in the definition of dtdzfn. A user



can redefine this function by making a copy of the source code and replacing the statements (in the copy) that correspond to the following:

```
if (zcm .le. 1600.01d+00) then
  dtdzfn = -0.1082d+00 / zcm
else
  dtdzfn = -0.2485d+00 / zcm
end if
```

#### CAUTION

##### Potential for Ruining Results

The common statements and the type declarations and values of the variables in any common statements must not be changed! Also, the type declaration (real\*8) and value of the formal parameter zcm must not be changed! Making such changes could lead to mismatches with other program units. Such mismatches could lead in turn to errors severe enough to ruin simulated data.

Local variables may be defined and used if none of their names are being used in common statements or as the formal parameter. Any newly defined variables should be declared in type statements (such as real\*8 or integer).

See section 7.2 for meanings of selected variables used in MACACASM.

### 3.22 If Error Message Is Encountered at This Point

For a certain type of conflict in input, the program may terminate abruptly at this point with the following error message:

STOP OOPS! Wrong height when trying to use subroutine devv\_get

If this error message is not encountered, skip to 3.23.

If this error message is produced, it probably results from a height value in file eff\_vert\_v.in being different from the current height being used by the Rachele-Kilmer microphysics model program after the user has specified that the effective vertical velocity is to be read from that file (method 2).

The heights in file `eff_vert_v.in` must agree (within a small tolerance) with the numerical integration height levels. The initial height given in the file must agree with the value entered via standard input for the initial height in meters above ground level (for example, 200 cm in file `eff_vert_v.in` agrees with 2 m entered via interactive input). Also, the difference in height values in consecutive lines in file `eff_vert_v.in` must agree with the value entered via standard input for the height increment in meters (for example, a 10 cm difference in the file agrees with 0.1 m entered via standard input).

If file `eff_vert_v.in` is produced by copying or renaming (using the `mv` command in UNIX) file `eff_vert_v.out` produced by a previous run of this same program, then either of two adjustments can be made to assure agreement. The preferred adjustment is to supply the appropriate standard input value for the initial (reference) height and the appropriate first number in the `.haze.defaults` file while repeating the run used to create the first `eff_vert_v.out` file. While repeating that run, choose method 3 to determine the effective vertical velocity. Also, the value entered via standard input for the initial height in meters above ground level should be identical to the corresponding value entered in subsequent runs. The first number in file `.haze.defaults` should be exactly 10,000 times the value entered via standard input for the height increment in meters (for example, 1000 and 0.1, respectively) in subsequent runs. (The tolerance allowed in testing agreement of heights is small - only 0.5 mm.) Copy the `eff_vert_v.out` output file to file `eff_vert_v.in` in the appropriate directory and use in subsequent runs.

The other adjustment that can be made is to repeat the run that produced the error message, but with one or two of the input values modified as necessary. Change one or both of the values entered via standard input for the initial height in meters above ground level and the height increment in meters to agree with the data already present in the `eff_vert_v.in` file.

If file `eff_vert_v.in` was produced by a method other than copying or renaming (`mv` command in UNIX) file `eff_vert_v.out` produced by a previous run of this same program, determine that the numbers in each line are in the expected order. The first number for each line is expected to be height (cm) above ground level, and the last of the three numbers in each line is expected to be

the effective vertical velocity (cm/s) of the cluster sphere. (The second number in each line is irrelevant, because it is read and ignored. However, some number must be present as a place holder in the second position. This seemingly strange requirement arose so that files `eff_vert_v.in` and `eff_vert_v.out` would be analogous: a copy of the latter file produced by one run of the program may be used with no change as the former file in a subsequent run. The second number in file `eff_vert_v.out` is the simulated total elapsed time used by the cluster sphere to rise from its initial height to its current height.)

### 3.23 Informative Message Concerning Expected Output Data

In typical use, it is desired that the cluster sphere would stop rising before reaching the user-specified height. The following message (with the appropriate number in place of 549) is written to inform the user how many simulated data points to expect if the simulated cluster sphere ascends the entire distance to the user-specified final height:

```
If this simulation continues throughout the entire user-specified
height range, 549 plot data points are to be saved in each of the
plotit files a*.zyy and for each size class in multiple-sizeclass files
hazedsim.seque and mode2_ndrops.s.
```

Unless method 1 or 2 was selected for specifying dry radii, skip to 3.26.

### 3.24 If Method 1 Was Selected for Specifying Dry Radii

The next prompt appears if method 1 (user specifies each dry radius and each number of droplets) was selected for specifying dry radii. Otherwise, skip to 3.25.

```
Enter each dry radius (in cm), or enter a negative
number at the first prompt to use default radii:
```

```
For droplet size 1, dry radius =
```

If a non-negative number is entered here, it is used as the dry radius for the first (smallest) size class, and values for all of the other dry radii and for

droplet concentrations for every one of the size classes at the initial height must be entered.

If a negative number is entered here, the dry radii and initial droplet concentrations are defined using default values, estimated from Meppen 80 Profile 10 at a height of approximately 56.98 m above ground level by assuming that the relative humidity was exactly 1.0000 at that height. It was assumed that the temperature was 271.4402864 K and the pressure was 1006.0164 mbar (hPa) at that height. If using this set of dry radii, it is best to specify that there are exactly 17 drop size classes, because the set of default dry radii comprise exactly 17 values.

Skip to 3.26.

### **3.25 If Method 2 Was Selected for Specifying Dry Radii**

The next prompt appears if method 2 (user specifies each droplet radius at reference height and each number of droplets, and the relative humidity at the reference height is to be used in calculating dry radii) was selected for specifying dry radii. Otherwise, skip to 3.26.

Enter each droplet radius (in cm) at reference height, or enter a negative number at the first prompt to use default radii:

For droplet size 1, droplet radius =

If a non-negative number is entered, it is used as the droplet radius for the first (smallest) size class at the initial height, and the user also is expected to enter values for all of the other droplet radii at the initial height and for droplet concentrations for every one of the size classes at the initial height.

If a negative number is entered here, the initial droplet radii and initial droplet concentrations are defined using default values, obtained from Meppen 80 Profile 10 at a height of approximately 2.03675 m above ground level. If using this set of droplet radii, it is best to specify that there are exactly 15 drop size classes, because this set of default droplet radii comprise exactly 15 values.

### 3.26 Some Informative Output

Some of the user-specified or accepted values are repeated in a message such as the following:

```
Nuc type          = 20
fo                = 0.95000000
Po (dynes/cm2)    = 1000000.0
Tr (degrees kelvin) = 288.68270
Tr' (degrees kelvin) = 288.15000
Height increment(cm) = 10.000000
```

Unless method 4 or 5 was selected for specifying dry radii, skip to 3.28.

### 3.27 If Method 4 or 5 Was Selected for Specifying Dry Radii

The next prompt appears only if method 4 or 5 (Duncan-Low or Shettle-Fenn distribution is used for droplet radii at reference height, boundaries of droplet size intervals are set by the user or calculated, and the relative humidity at the reference height is to be used in calculating dry radii) was selected for specifying dry radii. Otherwise, skip to 3.28.

```
Enter radii (in cm) that define boundaries
of the size classes at reference height, or enter a
negative number at the first prompt to use default radii:
Enter largest droplet radius (in cm)
in size class    1 →
```

A negative number typically is entered here. An algorithm in the computer program calculates the radii that define the boundaries of the size classes at the initial (reference) height. If a lower cutoff is used, the size classes, except the last (largest radius) one, span an equal range on a log of wet radius scale. A message, as follows, appears in the standard output:

```
Default bounds will be used.
For size class 1, the largest droplet radius = 5.591832E-07
```

### 3.28 Optional Scaling of Initial Volume of Condensed Matter

The user is informed of the volume of condensed matter at the initial (reference) height. Multiplying the value by one million gives an acceptable estimate of the initial liquid water content in grams per cubic meter. Unless the drop concentration has been read from a file, the user is asked whether this volume of condensed matter is acceptable.

The calculated volume of condensed matter, using the original numbers of droplets you submitted, is 1.41892075E-09 cm<sup>3</sup> per cm<sup>3</sup>.  
Is this volume of condensed matter acceptable?

Answer y or n. If this volume is not acceptable, the user is prompted to enter the desired volume of condensed matter in units of cubic centimeter per cubic centimeter.

Enter desired volume of condensed matter in cm<sup>3</sup> per cm<sup>3</sup> →

Each original number of droplets is multiplied by the constant (same for each droplet size class) required to change the liquid water content to the desired value. (Note that this is, in effect, the same type of adjustment performed if the user specifies one common divisor of the Shettle-Fenn parameters N1 and N2 while using method 5 for specifying dry radii.) An example of a message to a user who has requested that the volume of condensed matter be 1.0E-8 cubic cm per cubic centimeter at the initial height follows:

Each original number of droplets has been multiplied by a constant  
to make the volume of condensed matter at reference level =  
1.00000000E-08

### 3.29 Informative Output

The vertical gradient of the water vapor mixing ratio (labeled dq/dz in output) is written to standard output at appropriate intervals. An example of a set of the messages follows:

```
At z = 200.,    dq/dz = -1.3719224965186E-8
At z = 1200.,   dq/dz = -1.3440637797124E-8
At z = 2200.,   dq/dz = -1.3183242455061E-8
```

At z = 3200., dq/dz = -1.2932076797549E-8  
 At z = 4200., dq/dz = -1.2691344870049E-8  
 At z = 5200., dq/dz = -1.2467374660478E-8  
 At z = 6200., dq/dz = -1.2271683234876E-8  
 At z = 7200., dq/dz = -1.212747749984E-8  
 At z = 8200., dq/dz = -1.208742595402E-8  
 At z = 9200., dq/dz = -1.2295051673876E-8  
 At z = 10200., dq/dz = -1.3329802849208E-8  
 — Saturation occurs at or just below height = 105.8 m. —  
 At z = 11200., dq/dz = -2.1727937243866E-8  
 At z = 12200., dq/dz = -3.4338202784332E-8  
 At z = 13200., dq/dz = -3.1443183157762E-8  
 At z = 14200., dq/dz = -3.0569623958481E-8  
 At z = 15200., dq/dz = -3.006542870718E-8  
 At z = 16200., dq/dz = -2.965564127314E-8  
 At z = 17200., dq/dz = -2.9286023705114E-8  
 At z = 18200., dq/dz = -2.8937751480236E-8  
 At z = 19200., dq/dz = -2.8602475204665E-8  
 At z = 20200., dq/dz = -2.8275932222981E-8  
 At z = 21200., dq/dz = -2.7955726437958E-8  
 At z = 22200., dq/dz = -2.7640411384011E-8  
 At z = 23200., dq/dz = -2.7329063865713E-8  
 At z = 24200., dq/dz = -2.7021067494661E-8  
 At z = 25200., dq/dz = -2.671599493075E-8  
 At z = 26200., dq/dz = -2.6413540388721E-8  
 At z = 27200., dq/dz = -2.6113478990618E-8  
 At z = 28200., dq/dz = -2.581564146967E-8  
 At z = 29200., dq/dz = -2.5519897935889E-8  
 At z = 30200., dq/dz = -2.5226147240252E-8  
 At z = 31200., dq/dz = -2.493430983365E-8  
 At z = 32200., dq/dz = -2.4644323030055E-8  
 At z = 33200., dq/dz = -2.4356137903048E-8  
 At z = 34200., dq/dz = -2.4069717392609E-8  
 At z = 35200., dq/dz = -2.3785035444601E-8  
 At z = 36200., dq/dz = -2.3502076995477E-8  
 At z = 37200., dq/dz = -2.3220839093577E-8  
 At z = 38200., dq/dz = -2.2941333256936E-8  
 At z = 39200., dq/dz = -2.266358971489E-8  
 At z = 40200., dq/dz = -2.2387663931864E-8  
 At z = 41200., dq/dz = -2.2113614908308E-8  
 At z = 42200., dq/dz = -2.1840607912031E-8  
 At z = 43200., dq/dz = -2.1551052559254E-8  
 At z = 44200., dq/dz = -2.1036887118052E-8  
 At z = 45200., dq/dz = -1.8752436999865E-8  
 At z = 46200., dq/dz = -7.7180730178962E-9  
 At z = 47200., dq/dz = 2.9339963662882E-8  
 At z = 48200., dq/dz = 1.0714209560853E-7  
 At z = 49200., dq/dz = 1.9831668970619E-7  
 At z = 50010., dq/dz = 2.5081328678096E-7

END OF SIMULATION: Sphere is no longer rising at height = 500.20  
meters.

Change in number of points in plot data:

Expected: 549      Actual: 499



## 4. Files and Standard Input and Output

During a successful simulation, a number of output files are written into the connected directory. Many of the output files are written in plotit format. A file in plotit format is an ASCII file containing one or more plot data sets. The first line of each of the data sets begins with three integers in 3i5 format. The first integer is the number of data points in the data set, and the next two integers are the line type and symbol type to be used in plotting. The last integer may be followed by text on the same line. The first line is followed by one line for each data point. Each of the additional lines contains two floating point numbers, which are the values of the X and Y coordinates for one point.

In the following list, the name of the file is followed by a brief description of the contents of the file:

standard input - See 2.1.4 for an example.

standard output

haze.out - an output text file suitable for printing with a 132-column format.

mode2\_ndrops.s, status = NEW, access = SEQUENTIAL, form = UNFORMATTED - binary file for possible use by another program. The concentration of drops attributed to mode 2 are written into this file when the initial drop size distribution is bimodal. When combined, the information in this file and file hazedsim.seque enables construction of vertical profiles of drop size distributions for each of the two modes separately, as well as the overall vertical drop size distribution profile.

hazedsim.seque, status = NEW, access = SEQUENTIAL, form = UNFORMATTED - a binary output file to which height, drop radii and concentrations, and  $dr/dz$  data (where  $r$  is drop radius and  $z$  is height above ground level) are written. The information in this file is sufficient to define a vertical drop size distribution profile and can be used with a program such as EEC8wave (extinction\_etc\_coefficients\_for\_8\_wavelengths) (see 5.2)

and Mie efficiency factors to calculate simulated vertical profiles of extinction, backscatter, scattering, and absorption coefficients.

hazedsim.bin, access = SEQUENTIAL, form = UNFORMATTED - a relatively small binary output file that complements file hazedsim.seque. Included in the values that it contains are equivalent radii of the dry condensation nuclei.

aarhoa.zyy - an ASCII output file, not in plotit format. Every line of this file contains a pair of values for height (cm) above ground level and density of dry air (in cgs units) inside the cluster sphere.

eff\_vert\_v.in, status = OLD - file that must be available as an input file if the user specifies that the effective vertical velocity of cluster is to be read from file eff\_vert\_v.in. Each line should contain three floating-point numbers to be read as height (cm) above ground level, a value to be ignored, and the effective vertical velocity (cm/s) of the cluster.

eff\_vert\_v.out - an ASCII output file in which each line contains three floating-point values: height (cm) above ground level, elapsed time (s) since cluster started ascending from reference height, and effective vertical velocity (cm/s) of the cluster.

rdry+ndrops - an ASCII output file, in which the first line contains the number of size classes, a number representing the method used for calculating number of drops, and the density of dry air at reference level. The rest of the file contains the dry radii and the number of particles in each size class at the reference level.

envf.zyy - an ASCII output file in plotit format containing data simulated for relative humidity in the ambient environment versus height (m) above ground level. The ambient environment is outside of the cluster sphere but in its immediate vicinity and at the same height. Relative humidity values written to plot files (and used within this program) are on a scale on which saturation = exactly 1.

aadlnf.zyy - an ASCII output file in plotit format containing data simulated for the first derivative of the natural logarithm of relative humidity (in the cluster sphere) with respect to height (cm) above ground level versus height (m) above ground level.

aadqdz.zyy - an ASCII output file in plotit format containing data simulated for the first derivative of the water vapor mixing ratio (in the cluster sphere) with respect to height (cm) above ground level versus height (m) above ground level.

aadtdz.zyy - an ASCII output file in plotit format containing data simulated for the first derivative of temperature (K) (in the cluster sphere) with respect to height (cm) above ground level versus height (m) above ground level.

aaf.zyy - an ASCII output file in plotit format containing data simulated for the relative humidity (in the cluster sphere) versus height (m) above ground level.

aaq.zyy - an ASCII output file in plotit format containing data simulated for the mixing ratio for water vapor (in the cluster sphere) versus height (m) above ground level.

aat.zyy - an ASCII output file in plotit format containing data simulated for the temperature (K) (in the cluster sphere) versus height (m) above ground level.

amwtot.zyy - an ASCII output file in plotit format containing data simulated for the total volume of condensed matter ( $\text{cm}^3/\text{cm}^3$ , actually a volume ratio) (in the cluster sphere) versus height (m) above ground level. Although this total volume of condensed matter includes both water and material from condensation nuclei, and the density of droplets might not be exactly  $1.0000 \text{ g cm}^{-3}$ , it is often an acceptable approximation to multiply this total volume by one million and call the result liquid water content or mass loading in units of  $\text{g m}^{-3}$ . Immediately following the three integers in the first line is the dry volume, which is the  $\text{cm}^3$  that would be occupied by the condensation nuclei from droplets in one  $\text{cm}^3$  of space in the cluster sphere at the reference (initial) height if no water were present.

**pwater.zyy** - an ASCII output file in plotit format containing data simulated for the partial pressure of water vapor ( $\text{dyn/cm}^2$ ) (in the cluster sphere) versus height (m) above ground level.

**envT.zyy** - an ASCII output file in plotit format containing data simulated for the temperature (K) in the ambient environment versus height (m) above ground level.

**.haze.defaults**, status = OLD: See section 2.1.3 for an example. - The information in this file (if it exists) is used to set height intervals at which plot data and printed output are to be written. This file should contain two integers - one integer per line - to define the intervals at which (1) plot data are written into various output files and (2) data are written into file haze.out, which would be suitable for printing. Both of these values should be in units of 0.1 mm. If the file does not exist, the default values in the program are used. (In either case, the values are modified and used in such a way that both intervals are multiples of the height step size selected.)

**drop.conc.in**, status = OLD, access = SEQUENTIAL, form = UNFORMATTED - needed as an input file if the user has chosen to have drop concentrations read from a binary data file by choosing response 3 (read from binary data file drop.conc.in) to the question "Do you want the number of droplets per cubic centimeter (except as modified by droplets falling out) to be ...". If this input file is needed, it must contain one record for each height level, and the record must contain the height (cm) above ground level followed by the number of drops per  $\text{cm}^3$  for each size class in order starting with size class 1. If the height read from this file does not agree (within reasonable tolerance) with the height being modeled, the program terminates abruptly with an error message.

**envq.zyy** - an ASCII output file in plotit format containing data simulated for the specific humidity in the ambient environment versus height (m) above ground level.

**LWC.Knoll** - an ASCII output file in plotit format containing data simulated for the volume of condensed matter ( $\text{cm}^3/\text{m}^3$ ) contained in drops having radii between 0.25 and 23.5  $\mu\text{m}$  versus height (m) above ground level.

**zbase\_b\_c,in, status = OLD:** See sections 2.1.1 and 2.1.2 for examples. - an optional ASCII input file. Its use is strongly recommended to set the height (m) above ground level of the base of the inversion layer equal to the height above ground level supplied for the top of the cloud in interactive input. If file **zbase\_b\_c,in** exists, it is expected to contain 4 or 10 values - one value per line. The quantities expected in this file are, in order:

- (1) **zbase:** height (m) above ground level of the base of INVERSION in sphere lapse rate equation
- (2) **bhbeqn:** b in extra term in sphere lapse rate equation
- (3) **chbeqn:** c in extra term in sphere lapse rate equation
- (4) **alapslin:** coefficient of the difference z-zlow in sphere lapse rate equation  
→(The file may end here if the default value of zero is desired for every one of the remaining constants.)
- (5) **c1turb:** a form factor to multiply **KK1tur**
- (6) **c2turb:** a form factor to multiply **KK2tur**
- (7) **c3turb:** a form factor to multiply **KK3tur**
- (8) **KK1tur:** the turbulent transfer coefficient for momentum
- (9) **KK2tur:** the turbulent transfer coefficient for heat
- (10) **KK3tur:** the turbulent transfer coefficient for water vapor mixing ratio

**COMB.file, access = SEQUENTIAL, form = UNFORMATTED** - a binary file intended for internal use to store data temporarily. It remains available and can be used with a copy of subroutine **wfiles**, that reads stored data from an unformatted file **COMB.file** and writes the same data into individual files, most of which are in plotit format.

**compare\_Tdiffs** - an output text file (if created) in the form of a table comparing three sets of temperature differences  $T - T'$ , where  $T$  is the cluster temperature and  $T'$  is the ambient air temperature at the same height. The table headings would be:

Height (m)	Modeled T - T'	T - T' Calc using approx eq 21 with full dL/dz	T - T' calc using approx eq 21 with dL/dz from only drops in Knollenberg range
---------------	-------------------	---	---

bounds.dat, access = SEQUENTIAL, form = UNFORMATTED - a relatively small binary output file that contains two records. These records contain:

Record 1: nsizes

Record 2: (bound(j), j = 0, nsizes)

where nsizes (integer) is the number of drop size classes, and the bound array (of real\*8) contains the values used as boundaries of drop radii (cm) in the partitioning of the initial drop size distribution into size classes.

## **5. Simulation of Vertical Profiles of Extinction, Backscatter, Absorption, and Scattering Coefficients and Visibility**

Sometimes it is desired to simulate vertical profiles of extinction, backscatter, absorption, and scattering coefficients and visibility. Multiplying Mie efficiency factors for single spherical droplets of given composition and size by the product of the number concentration of droplets of that size and the geometric cross-sectional area per droplet and summing over all droplet sizes yields extinction, backscatter, absorption, and total scattering coefficients. The meteorological range (visibility) is the natural logarithm of 50, which is about 3.912, divided by the extinction coefficient for a wavelength of  $0.55 \mu\text{m}$ .

Vertical profiles of drop size distributions, simulated using MACACASM, can be used to supply the needed values of number concentration of droplets and geometric cross-sectional area per droplet. The data can be used with other software that uses or calculates the Mie efficiency factors necessary to generate the desired vertical profiles. Such software has been prepared for use with an HP 9000 computer. This software includes a pair of programs: `calc_and_store_Mie_efficiency_factors_for_pure_water` and `EEC8wave`. `Calc_and_store_Mie_efficiency_factors_for_pure_water` is used to calculate and store a very large number of Mie efficiency factors for later lookup and use. The factors may be used many times without being recalculated. `EEC8wave` is used to read the stored values of Mie efficiency factors and drop size distribution data simulated using MACACASM and calculate vertical profiles of extinction, backscatter, absorption, and scattering coefficients and visibility.

### **5.1 Program to Calculate and Store Mie Efficiency Factors**

The source code for `calc_and_store_Mie_efficiency_factors_for_pure_water` is stored in file `~nkilmer/sources/store_Mie_ef.f` at ARL West. Unless the files `Effic.Factors` and `+Effic.Factors` containing Mie efficiency factors as functions of droplet radius are available, use this program to create files. Use of this program involves a large amount of number crunching, and execution takes such a long time that this program should be run using at or batch. Following is an example of batch when the (compiled and loaded) executable file has been

stored as /home/u22/nkilmer/bin/store\_Mie\_ef.x. The following example shows text entered at HP-UX command level; therefore, control-D is used to indicate the end of the batch job commands:

```
batch
/home/u22/nkilmer/bin/store_Mie_ef.x
^D
```

Mie calculations [5] are used with the complex indices of refraction for pure water to generate a large number of values for efficiency factors as functions of droplet radius for eight wavelengths. After the efficiency factors are calculated, they are stored and used when needed. This procedure avoids repeating time-consuming Mie calculations, which would have to be done if changes in complex indices of refraction with droplet growth were considered. The very large increase in computational efficiency enables calculating for more closely spaced droplet sizes than would be otherwise feasible.

Parts of the code for the program were copied from parts of program AGAUS (dated 16-Sept-1987) and converted to double precision. The code used from AGAUS includes subroutines MIEGX and ANGLE, most of BLOCKDATA, and selected fragments from the main program. The resulting double precision version of subroutine MIEGX is used to do the Mie calculations.

Eight wavelengths - 0.55, 1.06, 3, 4, 5, 8, 10.6, and 12  $\mu\text{m}$  - are used. The real and imaginary parts of the index of refraction of pure water are used for each wavelength. These values are set automatically within the program. Mie efficiency factors are calculated for many sizes of pure water droplets. The radii of the droplets and the calculated Mie efficiency factors for the eight wavelengths are stored in two unformatted sequential files (Effic.Factors and +Effic.Factors) in the connected directory.



## 5.2 Program to Calculate Vertical Profiles of Extinction, Scattering, Backscatter, and Absorption Coefficients and Visibility

The source code for EEC8wave has been stored in file `~nkilmer/sources/extin_hp.f` at ARL West and is appropriate for use with HP 9000 systems. (The Cray version of the source code for this program has been stored as file `~nkilmer/sources/extinC8w,seq.f` at ARL West.) The name EEC8wave came from "Extinction Etc Coefficients for 8 WAVElengths." EEC8wave is used to calculate and write extinction, scattering, backscatter, and absorption coefficients and visibility as functions of height.

Extinction, scattering, backscatter, and absorption efficiency factors for eight wavelengths are read as functions of droplet radius from the `Effic.Factors` and `+Effic.Factors` files. Drop size distribution data are read from files written using the version of MACACASM that writes sequential binary files and is suitable for use on a Hewlett-Packard 9000 computer. The files expected from a previous execution of MACACASM are named `aaf.zyy` (an ASCII file), `hazedsim.bin`, `hazedsim.seque`, and `bounds.dat` (binary sequential files). These files must exist in the connected directory. (Program EEC8wave creates a temporary binary sequential file. The temporary file, `cross_sect.bin`, may be deleted after successful execution of the program.)

If any droplets are smaller than the sizes for which stored Mie efficiency factors exist, a double precision version of subroutine MIEGX from program AGAUS is used to calculate the additional efficiency factors. The subroutine is one of the parts of the code that were copied from parts of program AGAUS (dated 16-Sept-1987) and converted to double precision as was done for the program discussed in section 5.1.

EEC8wave uses the same eight wavelengths - 0.55, 1.06, 3, 4, 5, 8, 10.6, and 12  $\mu\text{m}$  - for which efficiency factors were calculated and stored using a previously mentioned program (discussed in section 5.1 and stored in file `~nkilmer/sources/store_Mie_ef.f`). The real and imaginary parts of the index

of refraction of pure water are used for each wavelength, and the values are set automatically within both programs.

Drop size distribution data from MACACASM are used to calculate bounds and total cross-sectional area for each drop size class. Bounds and cross-sectional area data are used with Mie efficiency factors to calculate extinction, backscatter, absorption, and scattering coefficients.

The smallest value allowed for any drop radius is  $0.004\ \mu\text{m}$ . One way to assure that the input data does not include any smaller droplet radii is to specify this value as the lower cutoff value for the dry particle radius when using MACACASM.

Drop radii and size class bounds at the reference height are used to calculate interpolating fractions for estimating bounds for each size class above the reference height. A simple scheme is used to apportion the total geometric cross-sectional area of droplets in a given size class. This scheme is analogous to subdividing a rectangle (the width of which represents the range of radii in a size class, as in a histogram) into skinnier rectangles. Calculated efficiency factors already exist for one representative radius of each of these skinny rectangles. Having a large number of subdivisions per size class leads to smooth vertical profiles of extinction, absorption, and backscatter coefficients.

Although cloud and subcloud droplets contain small amounts of matter from condensation nuclei, the complex indices of refraction for pure water are used as a very reasonable approximation. Use of complex indices of refraction for pure water has a definite advantage. The same complex indices of refraction can be used for all drops at all heights. Thus, one set of Mie calculation results obtained for very closely spaced intervals can be stored and used indefinitely, enabling calculation of very closely spaced Mie efficiency factors without requiring large amounts of computer time. With the luxury of very closely spaced Mie efficiency factors, a simple interpolation scheme, which is analogous to subdividing bars of a histogram into many more narrow bars, is adequate. With such closely spaced Mie efficiency factors, very smooth simulated data are obtained, even when backscatter is involved.

### **5.2.1 *Parameter to Be Supplied to Main Program***

The path name of the directory that is expected to contain the Effic.Factors and +Effic.Factors files that contain values for Mie efficiency factors as functions of droplet radii is sought as the parameter supplied to the main program. For example, if the executable file of this program is file extin\_hp.x in the connected directory and the path name of the directory containing values for Mie efficiency factors is /home/u22/nkilmer/Mie, an appropriate command to invoke the program would be:

```
extin_hp.x /home/u22/nkilmer/Mie
```

If the path name parameter is missing or blank and the two files are not found in the connected directory, the user is prompted to enter the path name. (All other input and output files are to be in the connected directory.) If responding to a prompt, do not enter any leading blanks before the path name. The path name may be the full path name or relative to the connected directory.

### **5.2.2 *Output Files***

The file names extinct.zyy, visib.zyy, scatter.zyy, backscat.zyy, and absorpt.zyy in the connected directory are reserved for output files. The program will abort if any of these files exist in the connected directory when the program is started.

Vertical profiles of simulated extinction, scattering, backscatter, and absorption coefficients are to be represented in output files extinct.zyy, scatter.zyy, backscat.zyy, and absorpt.zyy, respectively. The four files contain data for all eight of the wavelengths listed. The output file named visib.zyy is defined only for a wavelength of 0.55  $\mu\text{m}$ , because it contains simulated visibility (meteorological range) data. All output files are in plotit format. Each data set in these files represents a vertical profile for one wavelength. Each line that represents a data point gives a value of the quantity suggested by the file name (not including .zyy) followed by the height in meters. The first mentioned value is in units of km for visibility,  $\text{km}^{-1} \text{sr}^{-1}$  for a backscatter coefficient, or  $\text{km}^{-1}$  for an extinction, scattering, or absorption coefficient.

## 6. Other Selected Programs That Can Be Used With Output from MACACASM

The files `~nkilmer/sources/hp_maca_dsd.f` and `~nkilmer/sources/wrt_boundsHP.f` contain programs that can be used to enable writing ASCII files containing data that were written to binary (unformatted) files during execution of MACACASM. This capability could be helpful if the information is to be copied to a system of a type different from that on which the binary files were created.

### 6.1 Rewriting Drop Size Distribution Data

Program `get_dsd`, which is stored in file `~nkilmer/sources/hp_maca_dsd.f` (for an HP 9000 system), enables rewriting data from three binary sequential files previously written using MACACASM. (Similar programs stored as files `~nkilmer/sources/maca_dsd_seq.f` and `~nkilmer/sources/maca_dsd_10.m.f` could be used on a Cray system.) One ASCII file (`dsd.dat`) is written for possible archival storage of simulated vertical profiles of drop radius and drop number concentration for each size class. Drop radius versus  $z$  (height above ground level) data may be read directly from this file (`dsd.dat`) using `plotit`.

Because a very large file could be created if ASCII representations of all of the data were written in their full real\*8 precision, the precision of the numbers written in ASCII form is reduced considerably. Also, the units used for drop radii are changed from centimeters to micrometers, and lines are formatted so the output file is relatively compact for an ASCII file.

Three unformatted (binary) sequential files (`hazedsim.bin`, `hazedsim.seque`, and `mode2_ndrops.s`) should have been written using MACACASM and should be in the connected directory. The output ASCII file is to be named `dsd.dat`, and there must not be any other file having that name in the connected directory.

## 6.2 Rewriting Bounds of Drop Size Classes

The program stored in file `~nkilmer/sources/wrt_boundsHP.f` (for an HP 9000 system) enables rewriting data from an unformatted file named `bounds.dat`, which should have been written using `MACACASM` and should be in the connected directory. The data representing drop radii that define bounds of drop size classes at the reference (initial) height are written as an ASCII file to be named `bounds.ascii`. (A similar program stored as file `~kilmer/sources/write_bounds.f` could be used on a Cray system.)

## 7. Selected Programming Notes for MACACASM

This version uses real\*8 variables, which are double precision on an HP 9000 system. However, numerical sensitivity in function xmeax is so great that some REAL\*16 precision is required. Function xmeax is now defined as a REAL\*16 function, and there are some REAL\*16 variables in function expval and subroutine iduncan.

### 7.1 Files and Standard Input and Output

Integer variables are used for unit numbers for files and standard input and output to simplify changing unit numbers if such changes are needed for portability.

Some output data are saved in files for possible plotting or other subsequent treatment. Names of these files are included in this section.

The integer variable used for the unit number is followed by the name of the file in the following list: (Section 4 contains descriptions of files.)

stdin - standard input: See 2.1.4 for an example.

stdout - standard output

unit26 - file haze.out

unit27 - file mode2\_ndrops.s, status = NEW, access = SEQUENTIAL, form = UNFORMATTED

unit28 - file hazedsim.seque, status = NEW, access = SEQUENTIAL, form = UNFORMATTED

unit29 - file hazedsim.bin, access = SEQUENTIAL, form = UNFORMATTED

unit32 - file aarhoa.zyy

unit35 - file eff\_vert\_v.in, status = OLD

unit36 - file eff\_vert\_v.out

unit37 - file rdry+ndrops

unit39 - file envf.zyy

unit41 - file aadlnf.zyy

unit42 - file aadqdz.zyy

unit43 - file aadtdz.zyy

unit44 - file aaf.zyy

unit45 - file aaq.zyy

unit46 - file aat.zyy

unit47 - file amwtot.zyy

unit48 - file pwater.zyy

unit49 - file envT.zyy

unit52 - file .haze.defaults, status = OLD: See section 2.1.3 for an example.

unit53 - file drop.conc.in, status = OLD, access = SEQUENTIAL,  
form = UNFORMATTED

unit54 - file envq.zyy

unit57 - file LWC.Knoll

unit61 - file zbase\_b\_c.in, status = OLD: See sections 2.1.1 and 2.1.2 for examples.

unit64 - file COMB.file, access = SEQUENTIAL, form = UNFORMATTED

unit65 - file compare\_Tdiffs

unit72 - file bounds.dat, access = SEQUENTIAL,  
form = UNFORMATTED

## 7.2 Meanings of Selected Variables

- |          |   |
|----------|---|
| alapslin | - coefficient of the difference z-zlow in sphere lapse rate equation  |
| alphae   | - entrainment parameter (called $\alpha$ in dialogue with user)<br>→ If the entrainment parameter ALPHAE is positive, it will be used, and the Priestley parameters will be set to zero.<br>→ If ALPHAE is zero, the Priestley parameters will be used if present in file zbase_b_c.in.<br>→ Negative values are not allowed for ALPHAE.        |
| aTmTp    | a constant to be used in calculation of envT, the temperature in the ambient environment: This constant and the constant bTmTp are defined and used to calculate envT in such a way that the temperature difference (tzero - envT) is a linear function of height above ground level and becomes zero at the top of the cloud (where z = ztop). |
| awt      | - the threshold water activity, which is approximated (according to Hänel and Lehmann, [2]) as "that activity of water at which the volume of condensed water is equal to the volume of the dry material"   |



awtd	- the threshold water activity divided by $\Delta T$
bhbeqn	- b in extra term, which is effective near the cloud top, in cluster sphere lapse rate equation
bTmTp	- a constant to be used in calculation of $T_{env}$ , the temperature in the ambient environment (See $aTmTp$ .)
c1turb	- a form factor to multiply $KK1_{turb}$
c2turb	- a form factor to multiply $KK2_{turb}$
c3turb	- a form factor to multiply $KK3_{turb}$
chbeqn	- c in extra term, which is effective near the cloud top, in cluster sphere lapse rate equation
Cp	- heat capacity ( $\text{erg g}^{-1} \text{K}^{-1}$ ) of dry air at constant pressure
CpliqH2O	- specific heat of liquid water ( $\text{erg g}^{-1} \text{K}^{-1}$ )
Cpvapor	- heat capacity (constant pressure) of water vapor ( $\text{erg g}^{-1} \text{K}^{-1}$ )
deltat	- the curvature correction when the water activity equals the threshold water activity
denH2O	- density ( $\text{g cm}^{-3}$ ) of liquid water
direction	- real*8 variable that indicates the vertical direction of motion the simulated cluster sphere must take to go from starting height to ending height:  +1.0 => upward -1.0 => downward

This variable should have only the value +1.0 when set, because downward motion of the cluster sphere is not supported by this program.

- done - a logical variable used to indicate whether simulation is complete. When this variable equals .true., writing to output files will be completed, files will be closed, and execution will end.
- dqqdz -  $d(\text{mixing ratio})/dz$  at the level at which matrix equation is solved
- dryrad(j) - dry radius (cm) of condensation nucleus (when regarded as its equivalent sphere) for size class j
- dryrmin - smallest dry particle radius to be allowed (or 0.0 for no cutoff) (real\*8; input by user if not 0.0)
- dtdz -  $d(\text{temperature})/dz$  in cluster sphere: sometimes at the height level at which matrix equation is solved, and sometimes the mean of  $(\text{temperature})/dz$  values at two consecutive height levels
- dtdzmeth - method used to determine  $dT/dz$  (T is temperature in cluster sphere):
  - 1 - moist adiabatic approximation
  - 2 -  $dT/dz = \text{constant}$  defined by user
  - 3 - calculation from function dtdzfn
  - 201 - both  $dT/dz$  and mass loading initially are unknown in cluster sphere. An equation from thermodynamics and the ideal gas law is included to determine  $dT/dz$  and  $d(\text{water vapor mixing ratio})/dz$  as unknowns in this sphere.

<b>dtempdz</b>	- <b>d(temperature)/dz</b> at the height level the matrix equation is solved. This variable is never used to store the mean of <b>dT/dz</b> values at two consecutive levels. <b>dtdz</b> is used to store the latter quantity.
<b>eff_vert_v</b>	- <b>effective vertical velocity</b> of ascending cluster (cm/s). Sometimes <b>w</b> is used for this quantity.
<b>envdTdz</b>	- <b>vertical gradient of temperature</b> in ambient environment
<b>envmixrat</b>	- <b>mixing ratio</b> for water vapor in ambient environment at same height as cluster sphere
<b>envT</b>	- <b>temperature (K)</b> in ambient environment at same height as cluster sphere
<b>envTr</b>	- <b>temperature (K)</b> in ambient environment at reference (initial) height
<b>epsilon</b>	- <b>ratio of the molecular mass of water</b> to the mean molecular mass of dry air
<b>eta</b>	- <b>exponential mass increase coefficient</b>
<b>etazero</b>	- <b>value of eta</b> extrapolated for an infinitely dilute aqueous solution
<b>fall_out_of_sphere</b>	- <b>logical variable</b> used to indicate whether drops fall out of cluster sphere when their settling velocities exceed the ascent velocity of the sphere
<b>fallout(i)</b>	- <b>logical variable</b> used to indicate whether the droplets in size class <b>i</b> are present (if <b>.false.</b> ) or absent because of gravitational settling (if <b>.true.</b> )

<b>first</b>	- a logical variable used to indicate whether the simulated cluster sphere is still at its first (reference) height (if .true.) or at some other height (if .false.)
<b>fzero</b>	- relative humidity (1.0 = saturation) in cluster sphere
<b>grvcgs</b>	- acceleration due to gravity (cm sec <sup>-2</sup> )
<b>KK1tur</b>	- the turbulent transfer coefficient for momentum
<b>KK2tur</b>	- the turbulent transfer coefficient for heat
<b>KK3tur</b>	- the turbulent transfer coefficient for water vapor mixing ratio
<b>last_eq_size</b>	- last size class where droplets are always at their equilibrium sizes. The variable can be used if drops in a certain number of the smaller size classes are modeled as always being at their equilibrium sizes. In normal use of the program, all droplets exhibit diffusion-controlled growth and evaporation above the reference height; therefore, last_eq_size is set equal to 0.
<b>latentv</b>	- specific enthalpy of vaporization of water (erg g <sup>-1</sup> )
<b>lawco(j)</b>	- the coefficient of $rr^j$ (where $rr$ is the ratio of dry radius to wet radius) in the fitting polynomial used to calculate $\eta/\eta_{\text{zero}}$ as part of the calculation of the activity of water in a droplet
<b>lawncf</b>	- degree of fitting polynomial (in powers of the ratio of dry radius to wet radius) used to calculate $\eta/\eta_{\text{zero}}$ as part of the calculation of the activity of water in a droplet

- level** - number of current level (reference level = 1, etc.)
- meth\_for\_evap\_store** - method for determining effective vertical velocity of cluster sphere (integer chosen by user):

Effective vertical velocity of cluster is

- 1 - constant (value entered by user)
- 2 - read from file `eff_vert_v.in`
- 3 - calculated using cluster sphere buoyancy
- 4 - calculated as a linear function of height

- mixrat** - mixing ratio for water vapor in cluster sphere
- mwH2O** - molecular weight of water
- N1divisor** - constant used to divide Shettle-Fenn parameter N1 (real\*8; input by user if different from 1.0)
- N2divisor** - constant used to divide Shettle-Fenn parameter N2 (real\*8; input by user if different from 1.0)
- ndarray(j)** - number of droplets per cm<sup>3</sup> in size class j
- nodmode** - Number Of Drops MODE: integer input by user (integer used internally). The number of droplets/cm<sup>3</sup> (except possibly as modified by droplets falling out) are
- 1(1) - constant
  - 2(2) - proportional to the density of dry air
  - 3(6) - read from binary data file `drop.conc.in`
  - 4(8) - inversely proportional to cluster sphere volume, which depends on density in cluster sphere

<b>nsizes</b>	- number of droplet size classes
<b>nuctype</b>	- nucleus type (integer input by user)
<b>outplevel</b>	- level of output desired: <ul style="list-style-type: none"> <li>1 - data files only</li> <li>2 - data files plus some text (not much for each drop size class)</li> <li>3 - data files plus much text, including values for each size class</li> </ul>
<b>pdry</b>	- partial pressure ( $\text{dyn cm}^{-2}$ ) of dry air
<b>pdryref</b>	- partial pressure ( $\text{dyn cm}^{-2}$ ) of dry air at reference (initial) height
<b>pdynes</b>	- total pressure ( $\text{dyn cm}^{-2}$ )
<b>plot_interval</b>	- height interval at which plot data are written (Although initially in units of 0.1 mm, integer is converted to the exact number of height steps in the interval.)
<b>Pradius</b>	- radius (cm) of cluster sphere
<b>Pradref</b>	- radius (cm) of cluster sphere at reference height
<b>prelim</b>	- a logical variable used to indicate whether execution is in preliminary mode (.true. if in preliminary mode; .false. otherwise)
<b>pwater</b>	- partial pressure ( $\text{dyn cm}^{-2}$ ) of water vapor

pzero	- total pressure (mbar) (Although the total pressure at the initial height is accepted from the user in these units, the corresponding cgs variable, pdynes, is defined and used internally.)
radius(i)	- radius (cm) of drop in size class i
rdcgs	- specific gas constant ( $\text{erg g}^{-1} \text{K}^{-1}$ ) for dry air
regimc(j)	- regime of curvature correction for size class j (In some cases, different equations are appropriate for different regimes. The regimc array is used to communicate which curvature correction regime is in effect for each droplet size class.)
rhoacgs	- density of dry air ( $\text{g/cm}^3$ ) in cluster sphere
rhoaref	- density of dry air ( $\text{g/cm}^3$ ) in cluster sphere at reference (initial) height
Rvapor	- specific gas constant for water vapor ( $\text{erg g}^{-1} \text{K}^{-1}$ )
SFmodel	- an integer that indicates which Shettle-Fenn model is to be used (input by user):  1 - rural 2 - maritime 3 - urban
sigmaw	- surface tension of liquid water at 273.16 K
sizemode	- method of specifying dry radii:

- 1 - User specifies each dry radius and each number of droplets
- 2 - User specifies each droplet radius at reference (initial) height and each number of droplets
- 4 - Duncan-Low distribution used for droplet radii at reference height, and boundaries of droplet size intervals set by user or calculated
- 5 - Shettle-Fenn distribution used for droplet radii at reference height, and boundaries of droplet size intervals set by user or calculated

The relative humidity at reference height is used in calculating dry radii in methods 2, 4, and 5.

spechum	- specific humidity
spvolH2O	- specific volume (cm <sup>3</sup> ) of pure liquid water
thetam	- damp potential temperature
tzero	- temperature (K) in cluster sphere
visib	- visibility (km) at initial (reference) height
wplot	- a logical variable used to indicate whether current data are to be written as plot data
writ	- a logical variable used to indicate whether current data are to be written as text, usually into file haze.out
writ_interval	- height interval at which printed output is written as text, usually into file haze.out (Although initially in units of 0.1 mm, integer is converted to be the exact number of height steps in interval.)
z	- height (cm) above ground level



- zbase                   - height (cm) above ground level of the base of inversion in sphere lapse rate equation: It is recommended that the height be identical to ztop. (Note: If file zbase\_b\_c.in exists, then zbase is read from that file in units of meters and converted immediately to units of cm.)
  
- zhigh                   - user-specified final height (cm) above ground level for the simulated cluster sphere. (Note: If simulated cluster sphere stops rising before this height is attained, the last height level at which this cluster sphere is rising would be used as the final height modeled.) (Also note: User input values for zhigh, zinc, zlow, and ztop are read in units of meters and converted to units of cm.)
  
- zinc                    - height increment (step size) (cm)
  
- zlow                    - initial height (cm) above ground level for the simulated cluster sphere
  
- ztop                    - height of top of cloud (cm) above ground level: It is recommended that this height be identical to zbase.

Threshold values related to curvature correction include awt, awtd, and deltat, which are in common block /param3/. Definitions of these variables are included in the preceding list.

## 7.3 General Notes

### 7.3.1 *Frequency of Output*

If file .haze.defaults exists in the connected directory, the information in that file is used to set height intervals at which plot data and printed output are to be written. If the file is not present, default values are used to set the intervals. The default height interval at which plot data are written to various

files is 0.2 m. The default initial value for the associated variable, plot\_interval, is 2000 (units of 0.1 mm). The default height interval at which printed output is written to file haze.out, which would be suitable for printing, is 10 m. The default initial value for the associated variable, writ\_interval, is 100000 (units of 0.1 mm).

The two associated variables are modified in such a way that the plot and write intervals will be exact multiples of the height step size selected. The modified definition of each of these associated variables (plot\_interval and writ\_interval) will be the number of height steps (of length zinc) in the interval.

### **7.3.2 Default Values Used if File "zbase\_b\_c,in" Is Not Present**

If file zbase\_b\_c,in is not present in the connected directory, default values are used in place of the constants that would have been read from the file. The default values include these values for constants in the cluster sphere lapse rate equation:

zbase	=	2.55d+04	for base of inversion (cm)
bhbeqn	=	0.d+00	
chbeqn	=	4.d-04	
alapslin	=	0.d+00	

The default values effectively eliminate the terms in which bhbeqn, chbeqn, and alapslin occur.

Default values also include these values for Priestley-type form factors and turbulent transfer coefficients at the reference height:

clturb	=	0.d+00
c2turb	=	0.d+00
c3turb	=	0.d+00
KK1tur	=	0.d+00
KK2tur	=	0.d+00
KK3tur	=	0.d+00

### 7.3.3 *Specific Enthalpy of Vaporization of Water*

Specific enthalpy of vaporization of water (in units of  $\text{erg g}^{-1}$ ) is based on data given by Haar et al. [6] and is calculated according to this equation:

$$\text{latent hv} = 2.5005d+10 - 2.36d+07 * (tzero - 273.16d+00)$$

### 7.3.4 *Treatment of Mass Due to Nuclei*

The density of liquid water ( $\text{denH}_2\text{O}$ ) also is used as the density of droplets in calculating the liquid water concentration, although the droplets are not composed of pure water. The mass of the nuclei is included in calculating the liquid water content but is not included in calculating  $\text{Cpstar}$  and the liquid water mixing ratio (a variable named  $\text{water}$ ) in the cluster sphere.

### 7.3.5 *Determination of Size Distributions*

The simulated dry particle size (radius) distribution and/or the simulated drop size (wet radius) distribution inside a representative cluster sphere are determined at the reference (initial) height. Either ( $\text{sizmode } 1$ ) the dry particle size (radius) distribution is to be specified directly, or ( $\text{sizmode } 2, 4, \text{ or } 5$ ) the drop size (wet radius) distribution is to be specified and the dry particle size distribution is to be calculated assuming (for the reference height only) that the system is at equilibrium inside the cluster sphere.

If  $\text{sizmode}$  is 4 or 5, parameters are determined for the appropriate continuous drop size distribution, which is later partitioned into a discrete distribution with the requested (or default) number of size classes. After being determined, discrete drop sizes will be used with other reference height information (including relative humidity) and constants associated with the selected condensation nucleus type to calculate the dry particle size distribution.

When a Shettle-Fenn or Duncan-Low drop size distribution is selected, the high end of that distribution is retained. The lower cutoff corresponds to a dry particle radius specified by the user.

### **7.3.6    *Ensuring Valid Values at Reference Height***

To ensure calculating valid values at the reference height, the first complete execution of the predictor-corrector loop is performed without changing height. Flags are set to indicate that execution is in preliminary mode and to suppress storing plot data and printing while in preliminary mode.

### **7.3.7    *Drop Sedimentation***

If the user has answered yes to the question "Do drops fall out of cluster sphere when their settling velocities exceed the ascent velocity of this sphere?", the sedimentation velocities of drops are compared against the ascent velocity of the cluster sphere. Any droplet size class in which drops have sedimentation velocities greater than the ascent velocity of the cluster sphere are eliminated and are not restored for the remainder of the simulation. If any eliminated size class has a smaller index (sizeclass or i) than any retained size class, size classes still present with higher indices also are eliminated and a warning message is written. The program is terminated if all size classes are eliminated.

### **7.3.8    *Assuring That Final Height Conforms to User's Request***

The last height is to be exactly what the user has specified, although it might require using a smaller increment (zinc) for the final step.

### **7.3.9    *Temporary Data Storage***

Data are stored temporarily in a combined unformatted file so a number of individual ASCII files can be written in plotit format, which requires having the number of data points available when the first line is written. Near the end of execution of the program, data stored in the combined unformatted file are read and written into individual ASCII files.

### **7.3.10    *Temperature in the Ambient Environment***

Calculation of temperature in the ambient environment is based on specifying that the difference between temperatures in the cluster sphere and the ambient environment varies linearly with height from the value at the initial (reference) height to zero at the top of the cloud.

### **7.3.11    *Turbulence Effects***

Turbulence effects may be represented either by traditional entrainment expressions or by expressions like (and one analogous to) expressions given by Priestley. [4] Use the Priestley-type expressions or the traditional entrainment expressions involving the constant  $\alpha$ , but do not use both.

### **7.3.12    *Vertical Acceleration of Cluster Sphere***

The equation for vertical acceleration of the cluster sphere does not include a Coriolis force term, that would depend on the east-west component of wind velocity. One possible method of estimating the east-west velocity component uses similarity expressions above the reference height. However, it is intended that similarity theory not be used at all in this model.

### **7.3.13    *Radii of Droplets and Particles***

Radii are calculated as though droplets and dry nuclei were perfect spheres. The `dryrad` array stores radii of dry nuclei. The simple variable `rdry` is used for the dry nucleus of the current size class. The `radius` array stores radii of droplets. The simple variable `rwet` sometimes represents the radius of a droplet in the current size class and a related quantity (such as the droplet radius if it were in equilibrium).

The initial guess used when solving iteratively for a droplet radius is 1.25 times the dry radius in subroutine `solver`, which is used to calculate equilibrium droplet radii at the reference height. The initial guess is not always appropriate. The program may terminate prematurely if the lower cutoff dry radius is set to zero or a very small value.

A nonequilibrium  $dr/dz$  equation from Henry Rachele, [7] revised to incorporate modified hydrostatic approximation, is used for all droplet size classes for all heights above the reference height. There is no automatic changing of any size class from equilibrium to nonequilibrium, except that all size classes are considered to be in equilibrium at the reference height, and all size classes are considered to obey the nonequilibrium  $dr/dz$  equation above the reference height.

#### **7.3.14    *Units***

Centimeter-gram-second (cgs) units are used in this program. Pressures (represented by variables named *pdry*, *pdynes*, *pwater*, etc.) used in typical calculations are in units of  $\text{dyn cm}^{-2}$ .

#### **7.3.15    *Hydrostatic Approximation***

Hydrostatic approximation is based on values in the ambient environment outside of the cluster sphere but at the same height as the cluster sphere. No condensed matter is considered, and the variable *envmixrat* (instead of *mixrat*) influences the hydrostatic approximation.

### **7.4    Selected Subprograms**

#### **7.4.1    *Function curvcor***

Function *curvcor* calculates curvature correction and some related values.

#### **7.4.2    *Subroutine dcurvco***

Subroutine *dcurvco* calculates partial derivatives of the natural logarithm of curvature correction. Subroutine *rhfunc* should be called before subroutine *dcurvco* is called, because the value of *awtd* (the threshold water activity divided by *deltat*) that might be needed in subroutine *dcurvco*, is calculated in *curvcor*, a function that is used in *rhfunc*.

### 7.4.3 Subroutine *devv\_put*

Subroutine *devv\_put* stores reference height values for effective vertical velocity and its derivative with respect to height. If *meth\_for\_evv\_store* is 2, derivative of effective vertical velocity is stored for each height, although the values for the reference height and final height actually are calculated for the reference height plus one-half of a height increment and the final height minus one-half of a height increment, respectively.

### 7.4.4 Subroutine *DROGESUP*

Subroutine *DROGESUP* (DROplet Growth Equation SetUP) calculates the coefficients (*dqdz\_coeff* and *dt dz\_coeff*) of the vertical gradients of mixing ratio and temperature and the right hand side (*rhs*) of an equation involving the vertical gradient of the radius of a droplet of size class *sizeclass*. These values may be used in defining a row, the position of which is equal to the value of *sizeclass*, of a matrix equation when droplets in this size class exhibit diffusion-controlled (nonequilibrium) growth.

### 7.4.5 Subroutine *environ*

Subroutine *environ* calculates values in the ambient environment. It is assumed that (1) no condensed matter is in the ambient environment and (2) the total pressure (dry air plus water vapor) in the ambient environment is identical to the total pressure in the ascending cluster sphere. The relative humidity in the ambient environment is set equal to the relative humidity in that cluster sphere.

### 7.4.6 Subroutine *errfun*

Subroutine *errfun* calculates the error function and the complement of the error function according to Cody. [8] Its formal parameters are:

<i>x</i>	-	argument for <i>erf</i> or <i>erfc</i> (real*8; input)
<i>erf</i>	-	value of error function (real*8; output)
<i>erfc</i>	-	value of complement of error function (real*8; output)

which - indicates which result is calculated directly from a rational function (integer; output):

- 1 if erf is calculated directly (and erfc from erf)
- 2 if erfc is calculated directly (and erf from erfc)

#### **7.4.7 Subroutine *evv\_calc***

Subroutine *evv\_calc* calculates the sphere radius (*Pradius*) using the ratio of partial density of dry air (in the sphere) to that at the reference height. This calculation does not count any of the entrained matter as part of the sphere.

If appropriate (that is, if *meth\_for\_evv\_store* is 3 or 4), the sphere radius and other quantities are used to calculate *devvdz* (i.e.,  $dw/dz$ ), which is used to calculate *w* by numerical integration.

The formal parameters for subroutine *evv\_calc* are:

- z* - height (cm) (input)
- w* - effective vertical velocity of cluster (without including any turbulent fluctuations) (output; value is also put into labeled common)

#### **7.4.8 Function *expval***

The function *expval* (with formal parameters *n*, *r1cm*, and *r2cm*) determines the expectation value of  $r^n$  for the interval of *r* from *r1cm* to *r2cm*. The method includes evaluating closed-form solutions of sums of definite integrals of the Duncan-Low  $n(r)$  density function.

The formal parameters *r1cm* and *r2cm* are droplet radii in units of cm. Although these are passed unchanged to subroutine *iduncan*, the equivalent radii (*r1* and *r2*) in micrometers are used when passing values to function *xmeax*.



#### 7.4.9 Subroutine *getdrs*

Subroutine *getdrs* sets up a matrix equation that is solved for  $d-/dz$  for each size class,  $(1/f) df/dz$  sometimes (if at reference height or if entrainment is not considered), and  $dW_v/dz$  and/or  $dT/dz$  in cluster sphere. (Here,  $f$  represents relative humidity on a scale on which saturation is exactly 1,  $W_v$  represents water vapor mixing ratio in the cluster sphere, and  $T$  represents temperature (K) in the cluster sphere.) Subroutine *PADLIMES* does the solving. Calculated values are stored in the *drdz* array and the simple variables *dlndz* (if at reference height or if entrainment is not considered) and *dqdz* and/or *dtdz*.

If the current height is the reference height or entrainment is not considered,  $(1/f) df/dz$  is included as an unknown to be determined, and a form of the Clausius-Clapeyron equation is included in forming the matrix equation. If the current height is not the reference height and entrainment is considered,  $(1/f) df/dz$  is omitted from the list of unknowns, and the Clausius-Clapeyron equation is omitted. The variable *ntlpru* (Next To Last Previous Row Used) is defined to facilitate using much of the same code for both cases.

Unless at the reference height or in a situation where program terminates abruptly in this loop, subroutine *drogesup* must be called when  $i = 1$  (because some values calculated only when  $i = 1$  are also needed in subsequent calls).

#### 7.4.10 Subroutine *iduncan*

Subroutine *iduncan* (that has formal parameters *r1cm*, *r2cm*, *M2drops*, and *TotDrops*) determines the number of droplets per  $\text{cm}^3$  having radii between *r1cm* and *r2cm*. This is done by evaluating a closed-form solution to a sum of definite integrals of the Duncan-Low  $n(r)$  density function.

The formal parameters *r1cm* and *r2cm* are droplet radii in centimeters. The equivalent radii (*r1* and *r2*) in micrometers are used when passing values to function *xmeax*.

Formal parameters - output (real\*16):

M2drops - concentration of mode 2 drops (number per  $\text{cm}^3$ ) having radii between r1cm and r2cm

TotDrops - total concentration of drops (number per  $\text{cm}^3$ ) having radii between r1cm and r2cm

#### 7.4.11 Subroutine Illinois

Subroutine Illinois uses an Illinois iterative process (a modified Regula Falsi method) [9] for computing a solution of  $f(x) = \text{fgiven}$ .

Formal parameters:

- f - name of real\*8 function, which must be available as a separate routine (input)
- fgiven - given value of  $f(x)$  (input; real\*8)
- x - root of  $f(x) - \text{fgiven} = 0$  (output; real\*8)
- x0 and x1 - two approximations of x such that  $f(x0) - \text{fgiven}$  and  $f(x1) - \text{fgiven}$  are of opposite sign. (These values may be changed by routine.) (input; real\*8)
- delta - convergence criterion: If change in value of estimate of root is less than or equal to delta, then root is considered to be found. (input; real\*8)
- valid - validity flag (output; integer):
  - = -2 indicates solution was not found; cause unknown.
  - = -1 indicates error: This failure occurs when the input values of x0 and x1 are such that  $f(x0) - \text{fgiven}$  and  $f(x1) - \text{fgiven}$  have the same sign or are equal, and the routine's attempt to define acceptable initial estimates fails.
  - = 1 indicates valid solution.

#### **7.4.12 Subroutine Inpcbloc**

The cluster sphere radius is calculated without including entrained matter. The resulting value is stored as Pradius in common block /entrcomm/.

If the initial drop size distribution was a bimodal distribution, the mode 2 drop concentration in the current size class is calculated (if necessary) and written into a binary file for possible use by another program. This additional information can be used for further treatment of data if the complex indices of refraction for drops belonging to mode 2 are assumed to be different from those for drops belonging to mode 1.

If a drop radius decreases, it is not allowed to decrease by more than half of the difference between the current drop radius and the dry radius for this size class.

#### **7.4.13 Subroutine interg**

Subroutine interg (that has formal parameters x1, x2, xi, y1, y2, and yi) uses geometric interpolation to determine the value of yi for the point (xi,yi) when xi and the points (x1,y1) and (x2,y2) are given.

#### **7.4.14 Subroutine inter2**

Subroutine inter2 (that has formal parameters x1, x2, xi, y1, y2, and yi) uses linear interpolation after transformation of x values to determine the value of yi for the point (xi,yi) when xi and the points (x1,y1) and (x2,y2) are given. X values are transformed to  $s = \ln(1 - x^2)$  before linear interpolation is performed. Y values are not transformed.

#### **7.4.15 Subroutine inter3**

Subroutine inter3 (that has formal parameters x1, x2, xi, y1, y2, ya, yd, and yi) uses linear interpolation of transformed values to determine the value of yi for the point (xi,yi) when ya, yd, xi, and the points (x1,y1) and (x2,y2) are given. X values are transformed to  $s = \ln(1 - x^2)$  before linear interpolation

is performed. Y values are transformed to  $t = [(y - y_a)/y_d]^{1.8}$  before linear interpolation is performed. After linear interpolation is performed in (s,t) space, the interpolated value for t is subjected to an inverse transformation to obtain  $y_i$ .

#### 7.4.16 *Function lnxpval*

The real\*8 function lnxpval (that has formal parameters m, r1, and r2) returns the value of the definite integral from r1 to r2 of  $r^m n(r) dr$  divided by the expected number of drops in this interval, where  $n(r)$  is the bimodal lognormal density function with parameters given in common block /lognor/.

#### 7.4.17 *Subroutine lnndrops*

Subroutine lnndrops (that has formal parameters r1, r2, M2drops, and TotDrops) returns the value of the definite integral from r1 to r2 of  $n(r) dr$ , where  $n(r)$  is the bimodal lognormal density function with parameters given in common block /lognor/. Because N1 and N2 are included in appropriate calculations, the returned value for TotDrops is the expected total number concentration of droplets in the interval from radius = r1 to r2, and the returned value for M2drops is the expected part of that concentration attributed to droplets in mode 2 of the bimodal distribution.

#### 7.4.18 *Function LognMomt*

The real\*8 function LognMomt (that has formal parameters m, rmode, sigma  $\sigma$  in equation (1), rlow, and rhigh) returns the value of the definite integral from rlow to rhigh of  $r^m n(r) dr$ , where  $n(r)$  is the lognormal density function defined as

$$n(r) = \frac{\exp [-(\text{Log } r - \text{Log } r_{\text{mode}})^2 / (2\sigma^2)]}{(\text{Ln } 10) r \sigma \sqrt{2\pi}} \quad (1)$$

Ln is the natural logarithm function, and Log is the base 10 logarithm function.

#### **7.4.19    *Function LWCclip***

The real\*8 function LWCclip (that has formal parameters nodmode, nsizes, pi, and rhoacgs) returns the volume of condensed matter ( $\text{cm}^3/\text{m}^3$ ) contained in drops having radii between 0.25 and 23.5  $\mu\text{m}$ .

#### **7.4.20    *Function LWCdiscr***

The real\*8 function LWCdiscr (that has formal parameters nodmode, nsizes, pi, rhoacgs, and writ) returns the volume of condensed matter ( $\text{cm}^3/\text{cm}^3$ ) contained in all of the modeled drops.

#### **7.4.21    *Subroutine LWCgrad***

Subroutine LWCgrad calculates vertical gradients of total drop volume (liquid water content) for all drops and for only those drops having radii between 0.25 and 23.5  $\mu\text{m}$ , inclusive.

#### **7.4.22    *Subroutine ndropi***

Subroutine ndropi stores initial numbers of droplets in an array that will not be changed after initialization.

#### **7.4.23    *Subroutine PADLIMES***

During a given iteration for a given height level, a system of linear equations that can be expressed as a matrix equation, is generated. Subroutine PADLIMES (figure 1) solves the matrix equation. To increase efficiency, subroutine PADLIMES was tailored to take advantage of the characteristics of the matrix equations this subroutine is required to solve: a large part of the coefficient matrix in each of these equations is an identity matrix composed of the upper left-hand  $\text{nsizes} \times \text{nsizes}$  elements of the whole coefficient matrix.

#### **7.4.24 Subroutine *partiDSD***

Subroutine *partiDSD* partitions a continuous drop size distribution to define a discrete distribution. The discrete distribution is defined to have a finite number of size classes that are defined for sections that have default boundaries or boundaries set by user. A representative radius (mean volume radius) is calculated for each section. (This subroutine is used if *sizmode* is 4 or 5.)

#### **7.4.25 Function *pnormal***

The real\*8 function *pnormal* (that has one formal parameter, *t*) calculates the probability that a normally distributed variable with mean 0 and standard deviation 1 will have a value between negative infinity and *t*.

#### **7.4.26 Function *psatf***

The real\*8 function *psatf* (that has one formal parameter, *tzero*) uses a function from Lowe and Ficke [10] to calculate the saturation vapor pressure over water when *tzero*, the temperature (K), is given.

The range of validity for this function is from -50 to +50 °C.



#### **7.4.27    *Function r16toi***

The real\*16 function r16toi (that has formal parameters base and power) raises a real\*16 number to an integer power if the integer is small. Repeated multiplications are used in a way that preserves mathematically expected behavior of a real number (base) raised to an integer power (exponent):

If the base is positive

    The function returns a positive value.

If the base is negative

    And the exponent is even (including zero), the function returns a positive value.

    And the exponent is odd, the function returns a negative value.

If the base is zero

    And the exponent is positive, the function returns zero.

    And the exponent is negative or zero, the calling program is aborted with an error message.

Formal parameters

    base - base (real\*16)

    power - exponent (integer)

#### **7.4.28    *Function rhf***

The real\*8 function rhf (containing one formal parameter, radius) returns relative humidity as a function of droplet radius. Subroutine Illinois calls this function in the process of solving for the droplet radius when relative humidity is given.

#### **7.4.29    *Function rhfrdry***

The real\*8 function rhfrdry (containing one formal parameter, radry) returns relative humidity as a function of dry radius. The subroutine Illinois calls this



function in the process of solving for the dry radius when relative humidity is given.

#### **7.4.30    *Subroutine rhfunc***

Subroutine rhfunc returns relative humidity, activity of water, and curvature correction, given the radius of the droplet and other variables in common.

#### **7.4.31    *Subroutine setnab***

Subroutine setnab sets values of the parameters alpha1, alpha2, beta1, beta2, N1, and N2 (stored in labeled common) according to Duncan and Low. [11] The values used are appropriate when radius is expressed in micrometers. This subroutine has one formal parameter visib, which is the visibility in kilometers (real\*8). The value must be supplied by the calling program unit.

#### **7.4.32    *Subroutine setnrs***

Subroutine setnrs sets parameters for a bimodal lognormal distribution according to a rural, maritime, or urban aerosol model of Shettle and Fenn. [3]

Subroutine setnrs requires input values for all three formal parameters:

fzero        -   relative humidity (1 = saturated) (real\*8)  
visibility   -   meteorological range in km (real\*8)  
SFmodel    -   the Shettle-Fenn model used (integer):

1 - rural  
2 - maritime  
3 - urban

Subroutine setnrs uses the interpolation routines inter2, inter3, and interg.

#### 7.4.33 *Subroutine slapsrat*

Subroutine slapsrat defines a coefficient and the right-hand side for cluster sphere lapse rate equation. (The name of this subroutine comes from Sphere LAPSe RATE.)

In part 1, a few initial values are stored.

Part 2 calculates quantities in an equation that results from the first law of thermodynamics, the ideal gas law, a hydrostatic approximation for pressure, expressions involving entrainment, an expression intended to model (very roughly) diffusion involving air above the cloud, and a linear term that helps in curve fitting and might be considered to represent other effects. This equation is to be solved with others for vertical gradients experienced by the cluster sphere.

#### 7.4.34 *Subroutine solver*

Subroutine solver has formal parameters fgiven (real\*8), rwet (real\*8), and sizeclass (integer). Subroutine solver calls subroutine Illinois to compute the droplet radius (rwet) at which the relative humidity in equilibrium with the droplet's surface equals the input value of fgiven. The formal parameter sizeclass is the size class of the droplet.

#### 7.4.35 *Subroutine solvrd*

Subroutine solvrd has formal parameters rwet (real\*8), radry (real\*8), and sizeclass (integer). Subroutine solvrd calls subroutine Illinois to compute the dry particle radius (radry) for which the relative humidity in equilibrium with the surface of a droplet having a wet radius equal to the input value of rwet equals the relative humidity value of fzero, which is available through labeled common and is used as an input value. Again, the formal parameter sizeclass is the size class of the droplet. The variable rdry of the /params/ common block is set equal to the value determined for the formal parameter radry.

#### 7.4.36 Subroutine *wrfiles*

Subroutine *wrfiles* reads stored data from unformatted file COMB.file and writes the same data into individual files, most of which are in plotit format.

#### 7.4.37 Function *xmeax*

The real\*16 function *xmeax* (which has formal parameters *are8*, *m*, *x1re8*, and *x2re8*) returns the value of the definite integral from *x1re8* to *x2re8* of  $x^m \exp(\text{are8} \cdot x) dx$ . *Are8*, *x1re8*, and *x2re8* are real\*8. *m* is an integer. The value returned by this function is real\*16.

### 7.5 Modifications Needed for Use on a Cray System

Global differences between a version that runs on an HP 9000 system (this version) and one that runs on a Cray system should include:

<u>HP 9000</u>	<u>Cray</u>
dabs	abs
dexp	exp
dfloat	float
dlog	alog
dsign	sign
dsqrt	sqrt
sngl	-(omit)-

The changes are appropriate because REAL\*8 precision, used for most of the floating-point variables, is considered double precision when using Fortran 77 on an HP 9000 computer but is considered single precision when using Fortran 77 on a Cray computer. Floating-point constants are specified as single precision for the Cray version, such as by replacing d (in this version) with e (for Cray version). Floating-point constants in this version are expressed in a form that facilitates global substitution to change from double precision to single precision.

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## Acronyms and Abbreviations

ARL	Army Research Laboratory
ASCII	American Standard Code for Information Interchange
cgs	centimeter-gram-second
EEC8wave	Extinction Etc. Coefficients for 8 WAVElengths
HP	Hewlett-Packard
LN	natural logarithm of
MACACASM	Microphysics and Cluster Ascent Cloud and Subcloud Model
nm	nanometers
rhs	right-hand side
sr	steradian

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